Appendix C

In Vitro Data for Substances Tested in the HET-CAM Test Method

C1 Test Method Protocols used to Generate *In Vitro* Data C-3

C2 Data Sorted by Reference C-15

C3 Data Sorted by Substance for IS(A) Analysis Method.....C-53

C4 Data Sorted by Substance for IS(A)-10 Analysis Method.....C-63

C5 Data Sorted by Substance for IS(A)-100 Analysis Method.....C-69

C6 Data Sorted by Substance for IS(B) Analysis Method C-75

C7 Data Sorted by Substance for IS(A)-10 Analysis Method.....C-89

C8 Data Sorted by Substance for IS(A)-100 Analysis Method.....C-111

C9 Data Sorted by Substance for Q-Score Analysis Method C-139

C10 Data Sorted by Substance for S-Score Analysis Method C-149

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Appendix C1

Test Method Protocols used to Generate *In Vitro* Data

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	CEC (1991)	Gettings et al. (1991)	Bagley et al. (1992)	Gettings et al. (1994)	Vinardell and Macián (1994)
Hen Strain	Lohmann Selected Leghorn	Lohmann's Selected White Leghorn LSL	White Leghorn	White Leghorn	Leghorn SA31
Egg Criteria for Use	Weight range of eggs between 50 g and 60 g	Not Noted	Weight range of eggs between 50 g and 60 g	Not Noted	Not Noted
Egg Storage (Prior to use)	Not Noted	Not Noted	Not Noted	Not Noted	Not Noted
Incubation Temperature (^{0}C)	37.5 $\pm$ 0.5	Not Noted	37.5 $\pm$ 0.5	38	Not Noted
Relative Humidity (%)	62.5 $\pm$ 7.5	Not Noted	62.5 $\pm$ 7.5	60	Not Noted
Egg Rotation?	Yes	Not Noted	Yes	Yes	Not Noted
Checking Egg Viability	Eggs candled on Day 5 and every day thereafter; non-viable embryos removed	Not Noted	Not Noted	Candled on Day 9 and non-viable embryos removed	Not Noted
Incubation Period	10 Days	10 Days	10 Days	9 Days	10 Days
Procedure for Opening Egg	Egg shell was scratched around the air chamber with a rotating dentist saw blade and then pared off. The inner shell was removed and the CAM was layed open.	Not Noted	Egg shell around the air pocket was removed with a dental rotary saw	Eggshell was scratched around the air cells and a small aperture was opened.	Egg shell was scratched around the air cell by a dentist's rotary saw and then pared off. After removal of the inner membrane, the CAM was exposed.
Manipulation of CAM	Not Noted	Not Noted	Not Noted	Not Noted	Not Noted

	CEC (1991)	Gettings et al. (1991)	Bagley et al. (1992)	Gettings et al. (1994)	Vinardell and Macián (1994)
Investigator Defined Test Substance Classes	Chemicals from various chemical classes	Hydro-alcoholic formulations	Chemicals from various chemical classes, commercial products, and personal care products	Oil/water -based personal care formulations	Commercial disinfectants
Total Test Substances Evaluated	21	10	32	18	6
Test Substance Quantity or Volume	0.3 mL or 0.1 g	Not Noted	0.3 mL or 0.1 g	0.3 mL	0.3 mL
Test Substance Concentrations Tested	0.1% to 100%	Not Noted	Tested solutions at concentrations that were 10% of those tested *in vivo*	3 concentrations tested: threshold concentration, 10% solution, undiluted	Diluted or undiluted
Application of Solids to CAM	Placed directly on CAM	Not Noted	All tested substances appear to be solubilized	All tested substances appear to be solubilized	All tested substances appear to be solubilized
Preferred Solvent	Not Noted	Not Noted	Not Noted	Not Noted	Distilled water
Rinse after Test Substance Application?	Yes, for solids. 20 seconds after application of test substance, rinsed with 5 mL warm water or saline solution	Not Noted	20 seconds after test substance applied rinsed with 5 mL warm water	Not Noted	Not Noted
Evaluation Period	Up to 300 seconds after test substance applied	Not Noted	At 0.5, 2, and 5 minutes after test substance applied	Up to 300 seconds after test substance applied	Up to 300 seconds after test substance applied
Controls and Test Standards	Not Noted	Not Noted	Vehicle	Not Noted	0.1 M NaOH, 1% SDS, 0.9% NaCl, distilled water
Number of Control Eggs	Not Noted	Not Noted	2 eggs	Not Noted	2 eggs per substance
Replicate Eggs	Minimum 6 eggs	Not Noted	4 eggs	3 eggs per concentration tested	6 eggs
Number of Replicate Experiments	Not Noted	Not Noted	Not Noted	2	Not Noted
Endpoints Assessed	Hemorrhage, lysis, and coagulation	Hemorrhage, vascular lysis, coagulation	Hyperemia, hemorrhage, coagulation	Hemorrhage, coagulation, lysis	Hemorrhage, vasoconstriction, coagulation
Endpoint Evaluation	The starting second that each of the three endpoints is observed is recorded.	The starting second that each of the three endpoints is observed is recorded.	Numerical time-dependent scores for three endpoints.	Seconds for the three endpoints recorded (see Kalweit, 1990)	The starting second that each of the endpoints is observed is recorded

	CEC (1991)	Gettings et al. (1991)	Bagley et al. (1992)	Gettings et al. (1994)	Vinardell and Macián (1994)
Analysis Method	Irritation Index is calculated using the formula: (301-sec H)/300*5+(301-sec L)/300*7=(301-sec C)*9; where H=Hemorrhage, L=Lysis; C=Coagulation; sec=starting second	Two different analyses were used. Both calculated an irritation index using time (seconds) of appearance of hemorrhage vascular lysis, or coagulation. The differences between the two methods was in the particular calculations used.	Scores are totaled to give a single value (maximum of 21). Mean value of 4 eggs calculated for final value.	Calculation of an Irritation Score for each egg. Mean value of individual Irritation Scores calculated.	Irritancy Potential calculated using the formula: (301-sec H)/300*5+(301-sec v)/300*7=(301-sec C)*9; where H=Hemorrhage, V=vasoconstriction; C=Coagulation of protein or blood; sec=starting second
Classification Scheme	Not Noted	Not Noted	Not Noted	**Practically None**: 0-0.9; **Slight Irritation**: 1-4.9; **Moderate Irritation**: 5-9.9; **Strong Irritation**: 10-21	**Practically None**: 0-0.9; **Slight Irritation**: 1-4.9; **Moderate Irritation**: 5-8.9; **Strong Irritation**: 9 21
GLP Compliance?	Not Noted	Not Noted	Not Noted	Not Noted	Not Noted
Notes		Cites Luepke (1985) as basis for protocol used	Cites Luepke and Kemper (1986) as basis for protocol	Cites Luepke (1985) as basis for scoring scheme	Cites Ergatt/Frame Data Bank (1990) as basis for protocol and analysis method
				To study the effects of slow acting materials, CAM scored 15 and 30 minutes after application on range from 0 (no reactions) to 3 (strong reactions)	

	Balls et al. (1995) (Non-Transparent Substances)	Balls et al. (1995) (Transparent Substances)	Kojima et al. (1995)	Gettings et al. (1996) (HET-CAM I, II)	Gettings et al. (1996) (HET-CAM III)
Hen Strain	Not Noted	Not Noted	Not Noted	Lohmann's Selected White Leghorn	White Leghorn
Egg Criteria for Use	Not Noted	Not Noted	Not Noted	Not Noted	Not Noted
Egg Storage (Prior to use)	Not Noted	Not Noted	Not Noted	Not Noted	Not Noted
Incubation Temperature (^{0}C)	Not Noted	Not Noted	37.6	Not Noted	38 $\pm$ 0.5
Relative Humidity (%)	Not Noted	Not Noted	about 70	Not Noted	60 $\pm$ 5
Egg Rotation?	Not Noted	Not Noted	Yes, once per hour	Not Noted	Yes
Checking Egg Viability	Not Noted	Not Noted	Not Noted	Not Noted	Candled on Day 9 and returned to incubator in vertical position
Incubation Period	9 Days	9 Days	10 Days	10 Days	10 Days
Procedure for Opening Egg	Not Noted	Not Noted	A portion of the egg shell was removed and a drop of water was placed onto the shell membrane to avoid bleeding. Then the CAM was exposed with forceps.	Not Noted	Shell and inner shell membrane were removed around the area defined by the air cell
Manipulation of CAM	Not Noted	Not Noted	Not Noted	Not Noted	Not Noted

	Balls et al. (1995) (Non-Transparent Substances)	Balls et al. (1995) (Transparent Substances)	Kojima et al. (1995)	Gettings et al. (1996) (HET-CAM I, II)	Gettings et al. (1996) (HET-CAM III)
Investigator Defined Test Substance Classes	Chemicals selected from the ECETOC database (acids, acyl halides, alcohols, aldehye, alkalis, esters, hetercyclics, hydrocarbons, inorganic chemicals, ketones, organophosphates, pesticides, surfactants, misc.)	Chemicals selected from the ECETOC database (acids, acyl halides, alcohols, aldehye, alkalis, esters, hetercyclics, hydrocarbons, inorganic chemicals, ketones, organophosphates, pesticides, surfactants, misc.)	Surfactants, solvents, formaldehyde	Surfactant-based personal care formulations	Surfactant-based personal care formulations
Total Test Substances Evaluated	59	59	24	25	25
Test Substance Quantity or Volume	Not Noted	Not Noted	0.2 mL	0.3 mL	0.1 mL
Test Substance Concentrations Tested	Not Noted	Not Noted	10% solution	3 concentrations tested: threshold concentration, 10% solution, undiluted	10% solution
Application of Solids to CAM	Not Noted	Not Noted	All tested substances appear to be solubilized	All test substances appear to be in liquid form	All test substances appear to be in liquid form
Preferred Solvent	Not Noted	Not Noted	Not Noted	Not Noted	Not Noted
Rinse after Test Substance Application?	After 3 minute exposure	Not Noted	Yes, after 20 seconds test substance was rinsed with water	Not Noted	After 20 seconds, with a saline rinse
Evaluation Period	Within 30 seconds of rinsing	Up to 300 seconds after test substance applied	At 0.5, 2, and 5 minutes after test substance rinsed	Up to 300 seconds after test substance applied	At 0.5, 2, and 5 minutes after test substance rinsed
Controls and Test Standards	5% Texapon AV (internal reference standard)	5% Texapon AV (internal reference standard)	Not Noted	Not Noted	Not Noted
Number of Control Eggs	Not Noted	Not Noted	Not Noted	Not Noted	Not Noted
Replicate Eggs	6 eggs	6 eggs	4 eggs	3 eggs per concentration tested	Not Noted
Number of Replicate Experiments	Not Noted	Not Noted	Not Noted	Not Noted	Not Noted
Endpoints Assessed	Hemorrhage, lysis, coagulation	Hemorrhage, lysis, coagulation	Hyperemia, hemorrhage, coagulation	Hemorrhage, lysis, coagulation	Dilation, hemorrhage, coagulation
Endpoint Evaluation	Endpoints scored from 0 (no reaction) to 3 (strong reaction)	The starting second that each of the endpoints is observed is recorded	Not Noted	The starting second that each of the endpoints is observed is recorded (see Kalweit 1990)	Numerical time-dependent scores for three endpoints.

	Balls et al. (1995) (Non-Transparent Substances)	**Balls et al. (1995) (Transparent Substances)**	**Kojima et al. (1995)**	**Gettings et al. (1996) (HET-CAM I, II)**	**Gettings et al. (1996) (HET-CAM III)**
Analysis Method	Calculation of "S Score". "S Score" is calculated using the most sensitive endpoint (endpoint can change from chemical to chemical). The scores recorded for the most sensitive endpoint are summarized for the 6 eggs. (Maximum for 6 eggs is 18)	Computer program calculates an Irritation Index. Irritation Index Is used to calculate a "Q Score". "Q Score" is a comparison of the Irritation Index of a test chemical with that of the reference chemical. If the effect of test chemical is identical to reference, Q is 1.0. If effect of test chemical is less irritating, Q is lower. If effect of test chemical is more irritating, Q is higher.	Score was calculated based on the time of onset for each endpoint. Mean value of 4 eggs calculated.	Mean Irritation Score (IS; determined at 10% concentration) of 3 eggs is calculated. The Irritation Threshold Concentration (ITC; lowest concentration producing a slight reaction during observation period) is calculated.	Time-dependent scores were used to calculate a single value (maximum of 21).
Classification Scheme	**Non Irritation**: S < 6 ; **Moderately Irritating**: 6<= S <15; **Severely Irritating**: S ≥15	**Non Irritating**: Q < 1.5; **Moderately Irritating:** 1.5 < Q <2.0; **Severely Irritating**: Q < 2.0	Not Noted	**Irritant (According to FHSA)**: IS ≥ 5.1 or IS/ITC ≥ 3.0	**Irritant (According to FHSA)**: Score ≥ 4.83
GLP Compliance?	Yes	Yes	Not Noted	Not Noted	Not Noted
Notes			Cites Luepke (1985) and Luepke and Wallat (1985) as basis for scoring scheme and analysis method.		

	Gilleron et al. (1996)	Spielmann et al. (1996)	Gilleron et al. (1997)	Hagino et al. (1999)
Hen Strain	White Essex	Not Noted	White Essex	White Leghorn
Egg Criteria for Use	Eggs were 7 days old prior to start of incubation and weighed 60 ± 5 g	Not Noted	Eggs were 7 days old	Not Noted
Egg Storage (Prior to use)	Not Noted	Not Noted	Not Noted	Not Noted
Incubation Temperature (^{0}C)	37.0 ± 0.5	Not Noted	37 ± 0.5	37.6
Relative Humidity (%)	62.5 ± 1.5	Not Noted	52.5 ± 2.5	about 70
Egg Rotation?	Yes, with large ends upward for 9 days	Not Noted	Not Noted	Yes, once an hour
Checking Egg Viability	Not Noted	Not Noted	Not Noted	Not Noted
Incubation Period	10 Days	Not Noted	10 Days	10 Days
Procedure for Opening Egg	Eggs were candled and non-viable eggs were discarded. The airspace delimited by the inner membrane at the large end of the egg was marked. The eggshell was removed using a dentist's rotating saw blade. The inner membrane was moistened with 1.5-2.0 mL of 0.9% NaCl and the egg was returned to the incubator (at 37) for a maximum of 20 mins. After incubation, the NaCl solution was removed, using a vacuum pump, and the inner membrane was removed with forceps.	Not Noted	Not Noted	Portion of the egg shell above the air space was removed.
Manipulation of CAM	A test substance applicator (TSA), which is comprised of a perlon mesh (pore diameter = 63 micron) locked between two Teflon rings, was placed on the CAM	Not Noted	A test substance applicator (TSA) was placed on the CAM	Drop of water is placed on the membrane (to avoid capillary bleeding). A silicone rubber ring is placed on the CAM.

	Gilleron et al. (1996)	Spielmann et al. (1996)	Gilleron et al. (1997)	Hagino et al. (1999)
Investigator Defined Test Substance Classes	Chemicals from various chemical classes	Chemicals from various chemical classes	Chemicals from various chemical classes	Surfactant, polyols, color additives, organic salts, PABA derivative, esters, inorganic chemicals, alcohols, amines, alkanolamines, carboxylic acids
Total Test Substances Evaluated	46	200	60	39
Test Substance Quantity or Volume	0.3 mL or 0.3 g of test substance placed inside the TSA	Not Noted	0.3 mL or 0.3 g of test substance placed inside the TSA	0.2 mL (placed inside the rubber ring on the CAM). Solids (0.2 g) are reduced to a fine powder with a No. 200 sieve and placed inside a rubber ring on the CAM.
Test Substance Concentrations Tested	Undiluted	1-100% solutions tested	Not Noted	0.1, 1, 10, and 100%
Application of Solids to CAM	Placed inside TSA	All tested substances appear to be solubilized	Placed inside TSA	Placed inside rubber ring
Preferred Solvent	0.9% NaCl	0.9% NaCl or olive oil	Not Noted	Not Noted
Rinse after Test Substance Application?	TSA (which contains the test substance) is removed after 20 seconds	Yes, after 5 minutes (for substances that were insoluble in eater or oil and were colored).	TSA (which contains the test substance) is removed after 20 seconds	Yes, after 20 seconds with distilled water
Evaluation Period	Up to 300 seconds after test substance applied	Up to 300 seconds after test substance applied	Up to 300 seconds after test substance applied	At 0.5, 2, and 5 minutes after test substance applied
Controls and Test Standards	Positive Controls: benzalkonium chloride, dimethylformamide, imidazole	Not Noted	Not Noted	Not Noted
Number of Control Eggs	Not Noted	Not Noted	Not Noted	Not Noted
Replicate Eggs	3	Not Noted	Not Noted	4 eggs
Number of Replicate Experiments	3	Not Noted	Not Noted	Not Noted
Endpoints Assessed	Hemorrhage, lysis, coagulation	Hemorrhage, coagulation, lysis	Hemorrhage, lysis, coagulation	Hyperemia, hemorrhage, coagulation
Endpoint Evaluation	The starting second that each of the endpoints is observed is recorded	The starting second that each of the endpoints is observed is recorded	The starting second that each of the endpoints is observed is recorded	Numerical time-dependent scores for three endpoints.

	Gilleron et al. (1996)	Spielmann et al. (1996)	Gilleron et al. (1997)	Hagino et al. (1999)
Analysis Method	Irritation Index calculated using the formula: (301-sec H)/300*5+(301-sec L)/300*7=(301-sec C)*9; where H=Hemorrhage, L=Vessel Lysis; C=Coagulation; sec=starting second. Mean of 3 assays were calculated. Reproducibility also was assessed.	Irritation Score calculated ((301-sec H)/300*5+(301-sec L)/300*7=(301-sec C)*9; where H=Hemorrhage, L=Lysis; C=Coagulation; sec=starting second) for 10% solution calculated (IS10). Irritation Threshold (ITC; lowest concentration of a test substance to induce an irritant reaction on the CAM) calculated.	Irritation Index calculated using the formula: (301-sec H)/300*5+(301-sec L)/300*7=(301-sec C)*9; where H=Hemorrhage, L=Vessel Lysis; C=Coagulation; sec=starting second. Mean value and SEM of are calculated.	Not Noted
Classification Scheme	**Non Irritant**: 0-4.9; **Irritant**: 5.0-21	**BGA Classification Model: Non/Slight**: ITC > 10 and IS10 <16; **Moderate**: (1) ITC > 16 and IS10 > 16 or (2) ITC < 10 and IS10 < 16; **Irritant (R36)**: (1) ITC < 10 and IS10 > 16 or (2) ITC < 2.5 and IS10 < 16; **Severe (R41)**: (1) ITC $\leq$ 1% or (2) ITC between 1 and 2.5% and IS10 $\geq$ 16. **Proposed model using mtc10 (see notes below): R41**: mtc10 < 50 seconds.	**Non Irritant**: 0-4.9; **Irritant**: 5.0-21	Not Noted
GLP Compliance?	Not Noted	Yes	Not Noted	Not Noted
Notes		Cites Luepke (1985) as basis for protocol. Cites Kalweit (1990) and Spielmann (1991) as publishing the protocol used. Cites the standard protocol for the test method as InVitox Protocol.	Cites Gilleron 1996 as basis for protocol and analysis method	Cites Luepke 1985 as basis for scoring method
		Nine additional endpoints were conducted using the raw data and the IS and IT scores in this analysis. Of these the endpoints evaluated, that best correlated with in vivo classification was mtc10 (mean detection time for appearance of coagulation when using a 10% solution).		

Abbreviations: CAM = Chorioallantoic membrane, ECETOC = European Centre for Ecotoxicology and Toxicology of Chemicals, FHSA = Federal Hazardous Substances Act (1964), IS = Irritation score, IT = Irritation threshold concentration, NaCl = Sodium chloride, NaOH = Sodium hydroxide, SDS = Sodium dodecyl sulfate, Sec = seconds.

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Appendix C2

Data Sorted by Reference

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Substance Name	CASRN	Lab	*In Vitro* Conc. Tested	*In Vitro* Physical Form Tested	Purity (%)	Solubility*	pH	IS(A)[1]	IS(A) SD	IS(A) Classification	Overall IS(A) Classification	IS(B)[2]	IS(B) SD	IS(B) Classification	Overall IS(B) Classification	S-Score[3]	S-Score Classification	Overall S-Score Classification	Q-Score[4]	Q-Score Classification	Overall Q-Score Classification	IS(B)-10[5]	IS(B)-10 Class.	Overall IS(B)-10 Class.	IS(B)-100[6]	IS(B)-100 Class.	Overall IS(B)-100 Class.	Reference
Triethanolamine	102-71-6		10%	Solution	n.p.			10.75		Severe	Severe																	Bagley et al. (1992)
Triton X-100	9002-93-1		1%	Solution	n.p.			9		Severe	Severe																	Bagley et al. (1992)
Acetone	67-64-1	1	100%	Liquid	>99	water soluble													18.36	Severe								Balls et al. (1995)
Acetone	67-64-1	2	100%	Liquid	>99	water soluble													13.53	Severe								Balls et al. (1995)
Acetone	67-64-1	3	100%	Liquid	>99	water soluble													0.80	Nonirritant	Severe							Balls et al. (1995)
Acetone	67-64-1	4	100%	Liquid	>99	water soluble													10.31	Severe								Balls et al. (1995)
Ammonium nitrate	6484-52-2	1	100%	Solid	>99.9	water soluble													1.80	Moderate								Balls et al. (1995)
Ammonium nitrate	6484-52-2	3	100%	Solid	>99.9	water soluble													1.30	Nonirritant	Moderate							Balls et al. (1995)
Ammonium nitrate	6484-52-2	2	100%	Solid	>99.9	water soluble										18.00	Severe											Balls et al. (1995)
Ammonium nitrate	6484-52-2	4	100%	Solid	>99.9	water soluble										12.00	Moderate	Severe										Balls et al. (1995)
L-Aspartic acid	70-47-3	1	100%	Solid	95	water soluble													0.00	Nonirritant	Nonirritant							Balls et al. (1995)
L-Aspartic acid	70-47-3	2	100%	Solid	95	water soluble										1.00	Nonirritant											Balls et al. (1995)
L-Aspartic acid	70-47-3	3	100%	Solid	95	water soluble										2.00	Nonirritant	Moderate										Balls et al. (1995)
L-Aspartic acid	70-47-3	4	100%	Solid	95	water soluble										6.00	Moderate											Balls et al. (1995)
Benzalkonium chloride	8001-54-5	1	1%	Solution	98	surfactant													3.41	Severe								Balls et al. (1995)
Benzalkonium chloride	8001-54-5	2	1%	Solution	98	surfactant													5.00	Severe								Balls et al. (1995)
Benzalkonium chloride	8001-54-5	3	1%	Solution	98	surfactant													3.90	Severe	Severe							Balls et al. (1995)
Benzalkonium chloride	8001-54-5	4	1%	Solution	98	surfactant													4.39	Severe								Balls et al. (1995)
Benzalkonium chloride	8001-54-5	1	5%	Solution	98	surfactant													6.93	Severe								Balls et al. (1995)
Benzalkonium chloride	8001-54-5	2	5%	Solution	98	surfactant													4.43	Severe								Balls et al. (1995)
Benzalkonium chloride	8001-54-5	3	5%	Solution	98	surfactant													1.20	Nonirritant	Severe							Balls et al. (1995)
Benzalkonium chloride	8001-54-5	4	5%	Solution	98	surfactant													6.49	Severe								Balls et al. (1995)
Benzalkonium chloride	8001-54-5	1	10%	Solution	98	surfactant													6.09	Severe								Balls et al. (1995)
Benzalkonium chloride	8001-54-5	2	10%	Solution	98	surfactant													7.03	Severe								Balls et al. (1995)
Benzalkonium chloride	8001-54-5	3	10%	Solution	98	surfactant													3.10	Severe	Severe							Balls et al. (1995)
Benzalkonium chloride	8001-54-5	4	10%	Solution	98	surfactant													6.14	Severe								Balls et al. (1995)

Substance Name	CASRN	Lab	*In Vitro* Conc. Tested	*In Vitro* Physical Form Tested	Purity (%)	Solubility[a]	pH	IS(A)[1]	IS(A) SD	IS(A) Classification	Overall IS(A) Classification	IS(B)[2]	IS(B) SD	IS(B) Classification	Overall IS(B) Classification	S-Score[3]	S-Score Classification	Overall S-Score Classification	Q-Score[4]	Q-Score Classification	Overall Q-Score Classification	IS(B)-10[5]	IS(B)-10 Class.	Overall IS(B)-10 Class.	IS(B)-100[6]	IS(B)-100 Class.	Overall IS(B)-100 Class.	Reference
Benzoyl-L-tartaric acid	2743-38-6	1	100%	Solid	n.p.	water soluble										0.00	Nonirritant	Nonirritant										Balls et al. (1995)
Benzoyl-L-tartaric acid	2743-38-6	3	100%	Solid	n.p.	water soluble										4.00	Nonirritant											Balls et al. (1995)
Butyl acetate	123-86-4	1	100%	Liquid	99	water insoluble													1.55	Moderate	Moderate							Balls et al. (1995)
Butyl acetate	123-86-4	2	100%	Liquid	99	water insoluble													1.23	Nonirritant								Balls et al. (1995)
Butyl acetate	123-86-4	3	100%	Liquid	99	water insoluble													1.80	Moderate								Balls et al. (1995)
Butyl acetate	123-86-4	4	100%	Liquid	99	water insoluble													1.93	Moderate								Balls et al. (1995)
Gamma-butyrolactone	96-48-0	1	100%	Liquid	>99	water soluble													22.04	Severe	Severe							Balls et al. (1995)
Gamma-butyrolactone	96-48-0	2	100%	Liquid	>99	water soluble													6.64	Severe								Balls et al. (1995)
Gamma-butyrolactone	96-48-0	3	100%	Liquid	>99	water soluble													1.97	Moderate								Balls et al. (1995)
Gamma-butyrolactone	96-48-0	4	100%	Liquid	>99	water soluble													4.02	Severe								Balls et al. (1995)
Captan 90 concentrate	133-06-2	1	100%	Solid	90	water soluble										0.00	Nonirritant	Nonirritant										Balls et al. (1995)
Captan 90 concentrate	133-06-2	3	100%	Solid	90	water soluble										0.00	Nonirritant											Balls et al. (1995)
Captan 90 concentrate	133-06-2	4	100%	Solid	90	water soluble										6.00	Moderate											Balls et al. (1995)
4-Carboxybenzaldehyde	619-66-9	1	100%	Solid	95	water insoluble										0.00	Nonirritant	Moderate										Balls et al. (1995)
4-Carboxybenzaldehyde	619-66-9	2	100%	Solid	95	water insoluble										6.00	Moderate											Balls et al. (1995)
4-Carboxybenzaldehyde	619-66-9	3	100%	Solid	95	water insoluble										6.00	Moderate											Balls et al. (1995)
4-Carboxybenzaldehyde	619-66-9	4	100%	Solid	95	water insoluble										4.00	Nonirritant											Balls et al. (1995)
Cetylpyridinium bromide	140-72-7	1	0.10%	Solution	98	surfactant													2.43	Severe	Nonirritant							Balls et al. (1995)
Cetylpyridinium bromide	140-72-7	2	0.10%	Solution	98	surfactant													0.00	Nonirritant								Balls et al. (1995)
Cetylpyridinium bromide	140-72-7	3	0.10%	Solution	98	surfactant													1.00	Nonirritant								Balls et al. (1995)
Cetylpyridinium bromide	140-72-7	4	0.10%	Solution	98	surfactant													0.00	Nonirritant								Balls et al. (1995)
Cetylpyridinium bromide	140-72-7	1	6%	Solution	98	surfactant													2.34	Severe	Severe							Balls et al. (1995)
Cetylpyridinium bromide	140-72-7	2	6%	Solution	98	surfactant													2.42	Severe								Balls et al. (1995)
Cetylpyridinium bromide	140-72-7	3	6%	Solution	98	surfactant													1.30	Nonirritant								Balls et al. (1995)
Cetylpyridinium bromide	140-72-7	4	6%	Solution	98	surfactant													3.11	Severe								Balls et al. (1995)

Substance Name	CASRN	Lab	*In Vitro* Conc. Tested	*In Vitro* Physical Form Tested	Purity (%)	Solubility[a]	pH	IS(A)[1]	IS(A) SD	IS(A) Classification	Overall IS(A) Classification	IS(B)[2]	IS(B) SD	IS(B) Classification	Overall IS(B) Classification	S-Score[3]	S-Score Classification	Overall S-Score Classification	Q-Score[4]	Q-Score Classification	Overall Q-Score Classification	IS(B)-10[5]	IS(B)-10 Class.	Overall IS(B)-10 Class.	IS(B)-100[6]	IS(B)-100 Class.	Overall IS(B)-100 Class.	Reference
Cetylpyridinium bromide	140-72-7	1	10%	Solution	98	surfactant													2.71	Severe								Balls et al. (1995)
Cetylpyridinium bromide	140-72-7	2	10%	Solution	98	surfactant													2.73	Severe								Balls et al. (1995)
Cetylpyridinium bromide	140-72-7	3	10%	Solution	98	surfactant													1.80	Moderate	Severe							Balls et al. (1995)
Cetylpyridinium bromide	140-72-7	4	10%	Solution	98	surfactant													4.67	Severe								Balls et al. (1995)
Chlorhexidine	55-56-1	1	100%	Solid	99.5	water insoluble										3.00	Nonirritant											Balls et al. (1995)
Chlorhexidine	55-56-1	3	100%	Solid	99.5	water insoluble										6.00	Moderate	Moderate										Balls et al. (1995)
Chlorhexidine	55-56-1	4	100%	Solid	99.5	water insoluble										11.00	Moderate											Balls et al. (1995)
Cyclohexanol	108-93-0	1	100%	Liquid	97	water soluble													3.28	Severe								Balls et al. (1995)
Cyclohexanol	108-93-0	2	100%	Liquid	97	water soluble													4.48	Severe								Balls et al. (1995)
Cyclohexanol	108-93-0	3	100%	Liquid	97	water soluble													5.20	Severe	Severe							Balls et al. (1995)
Cyclohexanol	108-93-0	4	100%	Liquid	97	water soluble													6.69	Severe								Balls et al. (1995)
Dibenzyl phosphate	1623-08-1	1	100%	Solid	99.5	water insoluble										0.00	Nonirritant											Balls et al. (1995)
Dibenzyl phosphate	1623-08-1	2	100%	Solid	99.5	water insoluble										18.00	Severe											Balls et al. (1995)
Dibenzyl phosphate	1623-08-1	3	100%	Solid	99.5	water insoluble										0.00	Nonirritant	Severe										Balls et al. (1995)
Dibenzyl phosphate	1623-08-1	4	100%	Solid	99.5	water insoluble										15.00	Severe											Balls et al. (1995)
2,6-Dichlorobenzoyl chloride	4659-45-4	1	100%	Liquid	99	water insoluble													10.14	Severe								Balls et al. (1995)
2,6-Dichlorobenzoyl chloride	4659-45-4	2	100%	Liquid	99	water insoluble													8.81	Severe								Balls et al. (1995)
2,6-Dichlorobenzoyl chloride	4659-45-4	3	100%	Liquid	99	water insoluble													1.90	Moderate	Severe							Balls et al. (1995)
2,6-Dichlorobenzoyl chloride	4659-45-4	4	100%	Liquid	99	water insoluble													2.53	Severe								Balls et al. (1995)
2,2-Dimethylbutanoic acid	595-37-9	1	100%	Liquid	>99	water insoluble													14.05	Severe								Balls et al. (1995)
2,2-Dimethylbutanoic acid	595-37-9	2	100%	Liquid	>99	water insoluble													10.64	Severe								Balls et al. (1995)
2,2-Dimethylbutanoic acid	595-37-9	3	100%	Liquid	>99	water insoluble													11.70	Severe	Severe							Balls et al. (1995)
2,2-Dimethylbutanoic acid	595-37-9	4	100%	Liquid	>99	water insoluble													14.73	Severe								Balls et al. (1995)
2,5-Dimethylhexanediol	110-03-2	1	100%	Solid	99.5	water insoluble													2.07	Severe								Balls et al. (1995)
2,5-Dimethylhexanediol	110-03-2	3	100%	Solid	99.5	water insoluble													0.80	Nonirritant	Severe							Balls et al. (1995)
2,5-Dimethylhexanediol	110-03-2	2	100%	Solid	99.5	water insoluble										18.00	Severe											Balls et al. (1995)
2,5-Dimethylhexanediol	110-03-2	4	100%	Solid	99.5	water insoluble										18.00	Severe	Severe										Balls et al. (1995)

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Ethanol	64-17-5	1	100%	Liquid	n.p.	water soluble													6.45	Severe	Severe							Balls et al. (1995)
Ethanol	64-17-5	2	100%	Liquid	n.p.	water soluble													10.63	Severe								Balls et al. (1995)
Ethanol	64-17-5	3	100%	Liquid	n.p.	water soluble													1.47	Nonirritant								Balls et al. (1995)
Ethanol	64-17-5	4	100%	Liquid	n.p.	water soluble													5.95	Severe								Balls et al. (1995)
Ethyl acetate	141-78-6	1	100%	Liquid	99	water soluble													3.94	Severe	Severe							Balls et al. (1995)
Ethyl acetate	141-78-6	2	100%	Liquid	99	water soluble													1.87	Moderate								Balls et al. (1995)
Ethyl acetate	141-78-6	3	100%	Liquid	99	water soluble													0.90	Nonirritant								Balls et al. (1995)
Ethyl acetate	141-78-6	4	100%	Liquid	99	water soluble													3.37	Severe								Balls et al. (1995)
2-Ethyl-1-hexanol	104-76-7	1	100%	Liquid	99	water soluble													1.24	Nonirritant	Nonirritant							Balls et al. (1995)
2-Ethyl-1-hexanol	104-76-7	2	100%	Liquid	99	water soluble													0.61	Nonirritant								Balls et al. (1995)
2-Ethyl-1-hexanol	104-76-7	3	100%	Liquid	99	water soluble													1.00	Nonirritant								Balls et al. (1995)
2-Ethyl-1-hexanol	104-76-7	4	100%	Liquid	99	water soluble													3.12	Severe								Balls et al. (1995)
Ethyl-2-methylacetoacetate	609-14-3	1	100%	Liquid	ca. 97	water insoluble													2.40	Severe	Severe							Balls et al. (1995)
Ethyl-2-methylacetoacetate	609-14-3	2	100%	Liquid	ca. 97	water insoluble													2.51	Severe								Balls et al. (1995)
Ethyl-2-methylacetoacetate	609-14-3	3	100%	Liquid	ca. 97	water insoluble													1.10	Nonirritant								Balls et al. (1995)
Ethyl-2-methylacetoacetate	609-14-3	4	100%	Liquid	ca. 97	water insoluble													2.35	Severe								Balls et al. (1995)
Ethyl trimethyl acetate	3938-95-2	1	100%	Liquid	99	water insoluble													0.10	Nonirritant	Nonirritant							Balls et al. (1995)
Ethyl trimethyl acetate	3938-95-2	2	100%	Liquid	99	water insoluble													0.19	Nonirritant								Balls et al. (1995)
Ethyl trimethyl acetate	3938-95-2	3	100%	Liquid	99	water insoluble													0.30	Nonirritant								Balls et al. (1995)
Ethyl trimethyl acetate	3938-95-2	4	100%	Liquid	99	water insoluble													1.01	Nonirritant								Balls et al. (1995)
Fomesafen	72128-02-0	1	100%	Solid	97.5	water soluble										0.00	Nonirritant	Moderate										Balls et al. (1995)
Fomesafen	72128-02-0	2	100%	Solid	97.5	water soluble										9.00	Moderate											Balls et al. (1995)
Fomesafen	72128-02-0	3	100%	Solid	97.5	water soluble										6.00	Moderate											Balls et al. (1995)
Fomesafen	72128-02-0	4	100%	Solid	97.5	water soluble										6.00	Moderate											Balls et al. (1995)

Substance Name	CASRN	Lab	*In Vitro* Conc. Tested	*In Vitro* Physical Form Tested	Purity (%)	Solubility*	pH	IS(A)[1]	IS(A) SD	IS(A) Classification	Overall IS(A) Classification	IS(B)[2]	IS(B) SD	IS(B) Classification	Overall IS(B) Classification	S-Score[3]	S-Score Classification	Overall S-Score Classification	Q-Score[4]	Q-Score Classification	Overall Q-Score Classification	IS(B)-10[5]	IS(B)-10 Class.	Overall IS(B)-10 Class.	IS(B)-100[6]	IS(B)-100 Class.	Overall IS(B)-100 Class.	Reference
Glycerol	56-81-5	1	100%	Liquid	99.5	water soluble													0.08	Nonirritant	Nonirritant							Balls et al. (1995)
Glycerol	56-81-5	2	100%	Liquid	99.5	water soluble													1.24	Nonirritant								Balls et al. (1995)
Glycerol	56-81-5	3	100%	Liquid	99.5	water soluble													0.60	Nonirritant								Balls et al. (1995)
Glycerol	56-81-5	4	100%	Liquid	99.5	water soluble													1.22	Nonirritant								Balls et al. (1995)
Hexanol	111-27-3	1	100%	Liquid	98	water insoluble													5.01	Severe	Severe							Balls et al. (1995)
Hexanol	111-27-3	2	100%	Liquid	98	water insoluble													3.98	Severe								Balls et al. (1995)
Hexanol	111-27-3	3	100%	Liquid	98	water insoluble													1.80	Moderate								Balls et al. (1995)
Hexanol	111-27-3	4	100%	Liquid	98	water insoluble													4.71	Severe								Balls et al. (1995)
Imidazole	288-32-4	1	100%	Solid	99	water soluble													11.19	Severe	Severe							Balls et al. (1995)
Imidazole	288-32-4	3	100%	Solid	99	water soluble													3.50	Severe								Balls et al. (1995)
Imidazole	288-32-4	2	100%	Solid	99	water soluble										18.00	Severe	Severe										Balls et al. (1995)
Imidazole	288-32-4	4	100%	Solid	99	water soluble										18.00	Severe											Balls et al. (1995)
Isobutanol	78-83-1	1	100%	Liquid	99.9	water insoluble													4.59	Severe	Severe							Balls et al. (1995)
Isobutanol	78-83-1	2	100%	Liquid	99.9	water insoluble													3.58	Severe								Balls et al. (1995)
Isobutanol	78-83-1	3	100%	Liquid	99.9	water insoluble													1.20	Nonirritant								Balls et al. (1995)
Isobutanol	78-83-1	4	100%	Liquid	99.9	water insoluble													5.89	Severe								Balls et al. (1995)
Isopropanol	67-63-0	1	100%	Liquid	99.9	water soluble													11.90	Severe	Severe							Balls et al. (1995)
Isopropanol	67-63-0	2	100%	Liquid	99.9	water soluble													5.79	Severe								Balls et al. (1995)
Isopropanol	67-63-0	3	100%	Liquid	99.9	water soluble													1.80	Moderate								Balls et al. (1995)
Isopropanol	67-63-0	4	100%	Liquid	99.9	water soluble													4.36	Severe								Balls et al. (1995)
Maneb	12427-38-2	1	100%	Solid	90	water soluble													0.00	Nonirritant	Nonirritant							Balls et al. (1995)
Maneb	12427-38-2	3	100%	Solid	90	water soluble										0.00	Nonirritant	Nonirritant										Balls et al. (1995)
Methyl acetate	79-20-9	1	100%	Liquid	98	water soluble													1.88	Moderate	Severe							Balls et al. (1995)
Methyl acetate	79-20-9	2	100%	Liquid	98	water soluble													5.39	Severe								Balls et al. (1995)
Methyl acetate	79-20-9	3	100%	Liquid	98	water soluble													1.70	Moderate								Balls et al. (1995)
Methyl acetate	79-20-9	4	100%	Liquid	98	water soluble													3.15	Severe								Balls et al. (1995)

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Methyl cyanoacetate	105-34-0	1	100%	Liquid	99	water soluble													1.51	Moderate	Moderate							Balls et al. (1995)
Methyl cyanoacetate	105-34-0	2	100%	Liquid	99	water soluble													1.21	Nonirritant								Balls et al. (1995)
Methyl cyanoacetate	105-34-0	3	100%	Liquid	99	water soluble													1.00	Nonirritant								Balls et al. (1995)
Methyl cyanoacetate	105-34-0	4	100%	Liquid	99	water soluble													1.78	Moderate								Balls et al. (1995)
Methylcyclopentane	96-37-7	1	100%	Liquid	>99	water insoluble													0.18	Nonirritant	Nonirritant							Balls et al. (1995)
Methylcyclopentane	96-37-7	2	100%	Liquid	>99	water insoluble													1.22	Nonirritant								Balls et al. (1995)
Methylcyclopentane	96-37-7	3	100%	Liquid	>99	water insoluble													0.20	Nonirritant								Balls et al. (1995)
Methylcyclopentane	96-37-7	4	100%	Liquid	>99	water insoluble													8.09	Severe								Balls et al. (1995)
Methyl ethyl ketone	78-93-3	1	100%	Liquid	99	water soluble													5.83	Severe	Severe							Balls et al. (1995)
Methyl ethyl ketone	78-93-3	2	100%	Liquid	99	water soluble													3.89	Severe								Balls et al. (1995)
Methyl ethyl ketone	78-93-3	3	100%	Liquid	99	water soluble													2.50	Severe								Balls et al. (1995)
Methyl ethyl ketone	78-93-3	4	100%	Liquid	99	water soluble													6.17	Severe								Balls et al. (1995)
Methyl isobutyl ketone	108-10-1	1	100%	Liquid	98	water insoluble													2.29	Severe	Moderate							Balls et al. (1995)
Methyl isobutyl ketone	108-10-1	2	100%	Liquid	98	water insoluble													1.04	Nonirritant								Balls et al. (1995)
Methyl isobutyl ketone	108-10-1	3	100%	Liquid	98	water insoluble													1.50	Moderate								Balls et al. (1995)
Methyl isobutyl ketone	108-10-1	4	100%	Liquid	98	water insoluble													1.86	Moderate								Balls et al. (1995)
1-Naphthalene acetic acid, Na salt	61-31-4	1	100%	Solid	95	water soluble													3.84	Severe	Severe							Balls et al. (1995)
1-Naphthalene acetic acid, Na salt	61-31-4	3	100%	Solid	95	water soluble													4.90	Severe								Balls et al. (1995)
1-Naphthalene acetic acid, Na salt	61-31-4	2	100%	Solid	95	water soluble										18.00	Severe	Severe										Balls et al. (1995)
1-Naphthalene acetic acid, Na salt	61-31-4	4	100%	Solid	95	water soluble										18.00	Severe											Balls et al. (1995)
1-Naphthalene acetic acid	86-87-3	1	100%	Solid	99	water soluble										6.00	Moderate	Moderate										Balls et al. (1995)
1-Naphthalene acetic acid	86-87-3	2	100%	Solid	99	water soluble										13.00	Moderate											Balls et al. (1995)
1-Naphthalene acetic acid	86-87-3	3	100%	Solid	99	water soluble										0.00	Nonirritant											Balls et al. (1995)
1-Naphthalene acetic acid	86-87-3	4	100%	Solid	99	water soluble										4.00	Nonirritant											Balls et al. (1995)

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Octanol	111-87-5	1	100%	Liquid	>99	water insoluble													2.10	Severe								Balls et al. (1995)
Octanol	111-87-5	2	100%	Liquid	>99	water insoluble													1.00	Nonirritant								Balls et al. (1995)
Octanol	111-87-5	3	100%	Liquid	>99	water insoluble													1.80	Moderate	Moderate							Balls et al. (1995)
Octanol	111-87-5	4	100%	Liquid	>99	water insoluble													1.78	Moderate								Balls et al. (1995)
Parafluoraniline	371-40-4	1	100%	Liquid	99	water insoluble													5.25	Severe								Balls et al. (1995)
Parafluoraniline	371-40-4	2	100%	Liquid	99	water insoluble													4.46	Severe								Balls et al. (1995)
Parafluoraniline	371-40-4	3	100%	Liquid	99	water insoluble													1.90	Moderate	Severe							Balls et al. (1995)
Parafluoraniline	371-40-4	4	100%	Liquid	99	water insoluble													2.57	Severe								Balls et al. (1995)
Polyethylene glycol 400	25322-68-3	1	100%	Liquid	n.p.	surfactant													1.59	Moderate								Balls et al. (1995)
Polyethylene glycol 400	25322-68-3	2	100%	Liquid	n.p.	surfactant													0.72	Nonirritant								Balls et al. (1995)
Polyethylene glycol 400	25322-68-3	3	100%	Liquid	n.p.	surfactant													0.60	Nonirritant	Nonirritant							Balls et al. (1995)
Polyethylene glycol 400	25322-68-3	4	100%	Liquid	n.p.	surfactant													1.22	Nonirritant								Balls et al. (1995)
Potassium cyanate	590-28-3	1	100%	Solid	97	water soluble													2.17	Severe								Balls et al. (1995)
Potassium cyanate	590-28-3	3	100%	Solid	97	water soluble													2.50	Severe	Severe							Balls et al. (1995)
Potassium cyanate	590-28-3	4	100%	Solid	97	water soluble													6.07	Severe								Balls et al. (1995)
Potassium cyanate	590-28-3	2	100%	Solid	97	water soluble										18.00	Severe	Severe										Balls et al. (1995)
Promethazine HCl	58-33-3	1	100%	Solid	98	water soluble													3.20	Severe								Balls et al. (1995)
Promethazine HCl	58-33-3	3	100%	Solid	98	water soluble													3.00	Severe	Severe							Balls et al. (1995)
Promethazine HCl	58-33-3	2	100%	Solid	98	water soluble										18.00	Severe											Balls et al. (1995)
Promethazine HCl	58-33-3	4	100%	Solid	98	water soluble										18.00	Severe	Severe										Balls et al. (1995)
Pyridine	110-86-1	1	100%	Liquid	>99	water soluble													3.84	Severe								Balls et al. (1995)
Pyridine	110-86-1	2	100%	Liquid	>99	water soluble													7.76	Severe								Balls et al. (1995)
Pyridine	110-86-1	3	100%	Liquid	>99	water soluble													12.90	Severe	Severe							Balls et al. (1995)
Pyridine	110-86-1	4	100%	Liquid	>99	water soluble													10.44	Severe								Balls et al. (1995)
Quinacrine	69-05-6	1	100%	Solid	n.p.	water soluble										0.00	Nonirritant											Balls et al. (1995)
Quinacrine	69-05-6	3	100%	Solid	n.p.	water soluble										4.00	Nonirritant	Nonirritant										Balls et al. (1995)
Quinacrine	69-05-6	4	100%	Solid	n.p.	water soluble										3.00	Nonirritant											Balls et al. (1995)

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Sodium hydroxide	1310-73-2	1	1%	Solution	n.p.	water soluble													6.34	Severe	Severe							Balls et al. (1995)
Sodium hydroxide	1310-73-2	2	1%	Solution	n.p.	water soluble													6.17	Severe								Balls et al. (1995)
Sodium hydroxide	1310-73-2	3	1%	Solution	n.p.	water soluble													4.80	Severe								Balls et al. (1995)
Sodium hydroxide	1310-73-2	4	1%	Solution	n.p.	water soluble													4.36	Severe								Balls et al. (1995)
Sodium hydroxide	1310-73-2	1	10%	Solution	n.p.	water soluble													13.13	Severe	Severe							Balls et al. (1995)
Sodium hydroxide	1310-73-2	2	10%	Solution	n.p.	water soluble													7.82	Severe								Balls et al. (1995)
Sodium hydroxide	1310-73-2	3	10%	Solution	n.p.	water soluble													23.00	Severe								Balls et al. (1995)
Sodium hydroxide	1310-73-2	4	10%	Solution	n.p.	water soluble													9.82	Severe								Balls et al. (1995)
Sodium lauryl sulfate	151-21-3	1	3%	Solution	98	surfactant													2.68	Severe	Severe							Balls et al. (1995)
Sodium lauryl sulfate	151-21-3	2	3%	Solution	98	surfactant													1.62	Moderate								Balls et al. (1995)
Sodium lauryl sulfate	151-21-3	3	3%	Solution	98	surfactant													1.70	Moderate								Balls et al. (1995)
Sodium lauryl sulfate	151-21-3	4	3%	Solution	98	surfactant													2.46	Severe								Balls et al. (1995)
Sodium lauryl sulfate	151-21-3	1	15%	Solution	98	surfactant													2.86	Severe	Severe							Balls et al. (1995)
Sodium lauryl sulfate	151-21-3	2	15%	Solution	98	surfactant													2.34	Severe								Balls et al. (1995)
Sodium lauryl sulfate	151-21-3	3	15%	Solution	98	surfactant													1.80	Moderate								Balls et al. (1995)
Sodium lauryl sulfate	151-21-3	4	15%	Solution	98	surfactant													4.37	Severe								Balls et al. (1995)
Sodium oxalate	62-76-0	1	100%	Solid	>99	water soluble										0.00	Nonirritant	Moderate										Balls et al. (1995)
Sodium oxalate	62-76-0	2	100%	Solid	>99	water soluble										12.00	Moderate											Balls et al. (1995)
Sodium oxalate	62-76-0	3	100%	Solid	>99	water soluble										11.00	Moderate											Balls et al. (1995)
Sodium oxalate	62-76-0	4	100%	Solid	>99	water soluble										9.00	Moderate											Balls et al. (1995)
Sodium perborate	10486-00-7	1	100%	Solid	98.6	water soluble										0.00	Nonirritant	Nonirritant										Balls et al. (1995)
Sodium perborate	10486-00-7	3	100%	Solid	98.6	water soluble										0.00	Nonirritant											Balls et al. (1995)
Sodium perborate	10486-00-7	4	100%	Solid	98.6	water soluble										7.00	Moderate											Balls et al. (1995)
Tetraaminopyrimidine sulfate	5392-28-9	1	100%	Solid	97	water insoluble										0.00	Nonirritant	Nonirritant										Balls et al. (1995)
Tetraaminopyrimidine sulfate	5392-28-9	3	100%	Solid	97	water insoluble										0.00	Nonirritant											Balls et al. (1995)
Tetraaminopyrimidine sulfate	5392-28-9	4	100%	Solid	97	water insoluble										6.00	Moderate											Balls et al. (1995)

Substance Name	CASRN	Lab	*In Vitro* Conc. Tested	*In Vitro* Physical Form Tested	Purity (%)	Solubility[a]	pH	IS(A)[1]	IS(A) SD	IS(A) Classification	Overall IS(A) Classification	IS(B)[2]	IS(B) SD	IS(B) Classification	Overall IS(B) Classification	S-Score[3]	S-Score Classification	Overall S-Score Classification	Q-Score[4]	Q-Score Classification	Overall Q-Score Classification	IS(B)-10[5]	IS(B)-10 Class.	Overall IS(B)-10 Class.	IS(B)-100[6]	IS(B)-100 Class.	Overall IS(B)-100 Class.	Reference
Thiourea	62-56-6	1	100%	Solid	>99	water soluble													1.31	Nonirritant	Nonirritant							Balls et al. (1995)
Thiourea	62-56-6	3	100%	Solid	>99	water soluble													0.50	Nonirritant								Balls et al. (1995)
Thiourea	62-56-6	2	100%	Solid	>99	water soluble										18.00	Severe	Severe										Balls et al. (1995)
Thiourea	62-56-6	4	100%	Solid	>99	water soluble										13.00	Moderate											Balls et al. (1995)
Toluene	108-88-3	1	100%	Liquid	99	water soluble													3.18	Severe	Severe							Balls et al. (1995)
Toluene	108-88-3	2	100%	Liquid	99	water soluble													5.84	Severe								Balls et al. (1995)
Toluene	108-88-3	3	100%	Liquid	99	water soluble													2.90	Severe								Balls et al. (1995)
Toluene	108-88-3	4	100%	Liquid	99	water soluble													2.98	Severe								Balls et al. (1995)
Trichloroacetic acid	76-03-9	1	3%	Solution	n.p.	water soluble													18.76	Severe	Severe							Balls et al. (1995)
Trichloroacetic acid	76-03-9	2	3%	Solution	n.p.	water soluble													9.15	Severe								Balls et al. (1995)
Trichloroacetic acid	76-03-9	3	3%	Solution	n.p.	water soluble													9.90	Severe								Balls et al. (1995)
Trichloroacetic acid	76-03-9	4	3%	Solution	n.p.	water soluble													5.33	Severe								Balls et al. (1995)
Trichloroacetic acid	76-03-9	1	30%	Solution	n.p.	water soluble													14.39	Severe	Severe							Balls et al. (1995)
Trichloroacetic acid	76-03-9	2	30%	Solution	n.p.	water soluble													9.96	Severe								Balls et al. (1995)
Trichloroacetic acid	76-03-9	3	30%	Solution	n.p.	water soluble													13.10	Severe								Balls et al. (1995)
Trichloroacetic acid	76-03-9	4	30%	Solution	n.p.	water soluble													11.81	Severe								Balls et al. (1995)
Triton X-100	9002-93-1	1	5%	Solution	98	surfactant													2.66	Severe	Severe							Balls et al. (1995)
Triton X-100	9002-93-1	2	5%	Solution	98	surfactant													2.72	Severe								Balls et al. (1995)
Triton X-100	9002-93-1	3	5%	Solution	98	surfactant													1.40	Nonirritant								Balls et al. (1995)
Triton X-100	9002-93-1	4	5%	Solution	98	surfactant													2.20	Severe								Balls et al. (1995)
Triton X-100	9002-93-1	1	10%	Solution	98	surfactant													3.45	Severe	Severe							Balls et al. (1995)
Triton X-100	9002-93-1	2	10%	Solution	98	surfactant													1.71	Moderate								Balls et al. (1995)
Triton X-100	9002-93-1	3	10%	Solution	98	surfactant													1.70	Moderate								Balls et al. (1995)
Triton X-100	9002-93-1	4	10%	Solution	98	surfactant													2.40	Severe								Balls et al. (1995)

Substance Name	CASRN	Lab	*In Vitro* Conc. Tested	*In Vitro* Physical Form Tested	Purity (%)	Solubility[a]	pH	IS(A)[1]	IS(A) SD	IS(A) Classification	Overall IS(A) Classification	IS(B)[2]	IS(B) SD	IS(B) Classification	Overall IS(B) Classification	S-Score[3]	S-Score Classification	Overall S-Score Classification	Q-Score[4]	Q-Score Classification	Overall Q-Score Classification	IS(B)-10[5]	IS(B)-10 Class.	Overall IS(B)-10 Class.	IS(B)-100[6]	IS(B)-100 Class.	Overall IS(B)-100 Class.	Reference
Tween 20	9005-64-5	1	100%	Liquid	98	surfactant													0.39	Nonirritant	Nonirritant							Balls et al. (1995)
Tween 20	9005-64-5	2	100%	Liquid	98	surfactant													0.38	Nonirritant								Balls et al. (1995)
Tween 20	9005-64-5	3	100%	Liquid	98	surfactant													0.60	Nonirritant								Balls et al. (1995)
Tween 20	9005-64-5	4	100%	Liquid	98	surfactant													0.95	Nonirritant								Balls et al. (1995)
Acetic acid	64-19-7	2	100%	Liquid	>99							14.8		Severe	Severe													CEC (1991)
Acetic acid	64-19-7	3	100%	Liquid	>99							13.7		Severe														CEC (1991)
Acetic acid	64-19-7	4	100%	Liquid	>99							9.3		Severe														CEC (1991)
Acetic acid	64-19-7	2	10%	Solution	>99							20.2		Severe	Severe													CEC (1991)
Acetic acid	64-19-7	3	10%	Solution	>99							13.6		Severe														CEC (1991)
Acetic acid	64-19-7	4	10%	Solution	>99							10.2		Severe														CEC (1991)
Benzalkonium chloride	8001-54-5	2	100%	Unknown	n.p.							14.5		Severe	Severe													CEC (1991)
Benzalkonium chloride	8001-54-5	3	100%	Unknown	n.p.							13.1		Severe														CEC (1991)
Benzalkonium chloride	8001-54-5	5	100%	Unknown	n.p.							5.8		Moderate														CEC (1991)
Benzalkonium chloride	8001-54-5	6	100%	Unknown	n.p.							6.9		Moderate														CEC (1991)
Benzalkonium chloride	8001-54-5	7	100%	Unknown	n.p.							13.3		Severe														CEC (1991)
Brij 35	9002-92-0	1	100%	Solid	>99							2.3		Slight	Slight													CEC (1991)
Brij 35	9002-92-0	2	100%	Solid	>99							4.3		Slight														CEC (1991)
Brij 35	9002-92-0	3	100%	Solid	>99							12.9		Severe														CEC (1991)
Brij 35	9002-92-0	4	100%	Solid	>99							4.4		Slight														CEC (1991)
Brij 35	9002-92-0	5	100%	Solid	>99							3.8		Slight														CEC (1991)
Brij 35	9002-92-0	6	100%	Solid	>99							2.6		Slight														CEC (1991)
Brij 35	9002-92-0	7	100%	Solid	>99							4		Slight														CEC (1991)
Butanol	71-36-3	1	100%	Liquid	99							11.7		Severe	Severe													CEC (1991)
Butanol	71-36-3	2	100%	Liquid	99							11.8		Severe														CEC (1991)
Butanol	71-36-3	3	100%	Liquid	99							12.6		Severe														CEC (1991)
Butanol	71-36-3	4	100%	Liquid	99							11.2		Severe														CEC (1991)
Butanol	71-36-3	5	100%	Liquid	99							3.9		Slight														CEC (1991)
Butanol	71-36-3	6	100%	Liquid	99							10.7		Severe														CEC (1991)
Butanol	71-36-3	7	100%	Liquid	99							9.9		Severe														CEC (1991)
Butanol	71-36-3	2	10%	Solution	99							14.2		Severe														CEC (1991)

Substance Name	CASRN	Lab	*In Vitro* Conc. Tested	*In Vitro* Physical Form Tested	Purity (%)	Solubility[a]	pH	IS(A)[1]	IS(A) SD	IS(A) Classification	Overall IS(A) Classification	IS(B)[2]	IS(B) SD	IS(B) Classification	Overall IS(B) Classification	S-Score[3]	S-Score Classification	Overall S-Score Classification	Q-Score[4]	Q-Score Classification	Overall Q-Score Classification	IS(B)-10[5]	IS(B)-10 Class.	Overall IS(B)-10 Class.	IS(B)-100[6]	IS(B)-100 Class.	Overall IS(B)-100 Class.	Reference
Butanol	71-36-3	3	10%	Solution	99							4.8		Slight	Severe													CEC (1991)
Butanol	71-36-3	4	10%	Solution	99							12.5		Severe														CEC (1991)
2-Butoxyethyl acetate	112-07-2	1	100%	Liquid	99							4.6		Slight														CEC (1991)
2-Butoxyethyl acetate	112-07-2	2	100%	Liquid	99							5.3		Moderate														CEC (1991)
2-Butoxyethyl acetate	112-07-2	3	100%	Liquid	99							4.7		Slight														CEC (1991)
2-Butoxyethyl acetate	112-07-2	4	100%	Liquid	99							4.7		Slight	Slight													CEC (1991)
2-Butoxyethyl acetate	112-07-2	5	100%	Liquid	99							4		Slight														CEC (1991)
2-Butoxyethyl acetate	112-07-2	6	100%	Liquid	99							3.9		Slight														CEC (1991)
2-Butoxyethyl acetate	112-07-2	7	100%	Liquid	99							4.5		Slight														CEC (1991)
2-Butoxyethyl acetate	112-07-2	2	10%	Solution	99							4.1		Slight														CEC (1991)
2-Butoxyethyl acetate	112-07-2	3	10%	Solution	99							0		Nonirritant	Slight													CEC (1991)
2-Butoxyethyl acetate	112-07-2	4	10%	Solution	99							3.2		Slight														CEC (1991)
Dibutyltin chloride	683-18-1	1	100%	Solid	97							11.6		Severe														CEC (1991)
Dibutyltin chloride	683-18-1	2	100%	Solid	97							10.8		Severe														CEC (1991)
Dibutyltin chloride	683-18-1	4	100%	Solid	97							12.6		Severe														CEC (1991)
Dibutyltin chloride	683-18-1	5	100%	Solid	97							5.1		Moderate	Severe													CEC (1991)
Dibutyltin chloride	683-18-1	6	100%	Solid	97							5		Moderate														CEC (1991)
Dibutyltin chloride	683-18-1	7	100%	Solid	97							13		Severe														CEC (1991)
Dimethyl sulfoxide	67-68-5	1	100%	Liquid	99.9							11.7		Severe														CEC (1991)
Dimethyl sulfoxide	67-68-5	2	100%	Liquid	99.9							10.9		Severe														CEC (1991)
Dimethyl sulfoxide	67-68-5	3	100%	Liquid	99.9							11.3		Severe														CEC (1991)
Dimethyl sulfoxide	67-68-5	4	100%	Liquid	99.9							4.1		Slight	Severe													CEC (1991)
Dimethyl sulfoxide	67-68-5	5	100%	Liquid	99.9							4.9		Slight														CEC (1991)
Dimethyl sulfoxide	67-68-5	6	100%	Liquid	99.9							7.3		Moderate														CEC (1991)
Dimethyl sulfoxide	67-68-5	7	100%	Liquid	99.9							11.4		Severe														CEC (1991)

Substance Name	CASRN	Lab	*In Vitro* Conc. Tested	*In Vitro* Physical Form Tested	Purity (%)	Solubility[a]	pH	IS(A)[1]	IS(A) SD	IS(A) Classification	Overall IS(A) Classification	IS(B)[2]	IS(B) SD	IS(B) Classification	Overall IS(B) Classification	S-Score[3]	S-Score Classification	Overall S-Score Classification	Q-Score[4]	Q-Score Classification	Overall Q-Score Classification	IS(B)-10[5]	IS(B)-10 Class.	Overall IS(B)-10 Class.	IS(B)-100[6]	IS(B)-100 Class.	Overall IS(B)-100 Class.	Reference
Dimethyl sulfoxide	67-68-5	2	10%	Solution	99.9							4.4		Slight														CEC (1991)
Dimethyl sulfoxide	67-68-5	3	10%	Solution	99.9							4.1		Slight	Slight													CEC (1991)
Dimethyl sulfoxide	67-68-5	4	10%	Solution	99.9							4.1		Slight														CEC (1991)
Glycerol	56-81-5	1	100%	Liquid	>99							10.8		Severe														CEC (1991)
Glycerol	56-81-5	2	100%	Liquid	>99							11.3		Severe														CEC (1991)
Glycerol	56-81-5	3	100%	Liquid	>99							10.3		Severe														CEC (1991)
Glycerol	56-81-5	4	100%	Liquid	>99							4.8		Slight	Severe													CEC (1991)
Glycerol	56-81-5	5	100%	Liquid	>99							0		Nonirritant														CEC (1991)
Glycerol	56-81-5	6	100%	Liquid	>99							0		Nonirritant														CEC (1991)
Glycerol	56-81-5	7	100%	Liquid	>99							9.4		Severe														CEC (1991)
Glycerol	56-81-5	2	10%	Solution	>99							8.7		Moderate														CEC (1991)
Glycerol	56-81-5	3	10%	Solution	>99							4.4		Slight	Slight													CEC (1991)
Glycerol	56-81-5	4	10%	Solution	>99							3.6		Slight														CEC (1991)
n-Hexane	110-54-3	1	100%	Liquid	99							2.9		Slight														CEC (1991)
n-Hexane	110-54-3	2	100%	Liquid	99							5.4		Moderate														CEC (1991)
n-Hexane	110-54-3	3	100%	Liquid	99							4.2		Slight														CEC (1991)
n-Hexane	110-54-3	4	100%	Liquid	99							10.3		Severe	Slight													CEC (1991)
n-Hexane	110-54-3	5	100%	Liquid	99							2.3		Slight														CEC (1991)
n-Hexane	110-54-3	6	100%	Liquid	99							8.1		Moderate														CEC (1991)
n-Hexane	110-54-3	7	100%	Liquid	99							2.4		Slight														CEC (1991)
n-Hexane	110-54-3	2	10%	Solution	99							3.7		Slight														CEC (1991)
n-Hexane	110-54-3	3	10%	Solution	99							0		Nonirritant	Severe													CEC (1991)
n-Hexane	110-54-3	4	10%	Solution	99							10.1		Severe														CEC (1991)

Substance Name	CASRN	Lab	*In Vitro* Conc. Tested	*In Vitro* Physical Form Tested	Purity (%)	Solubility[a]	pH	IS(A)[1]	IS(A) SD	IS(A) Classification	Overall IS(A) Classification	IS(B)[2]	IS(B) SD	IS(B) Classification	Overall IS(B) Classification	S-Score[3]	S-Score Classification	Overall S-Score Classification	Q-Score[4]	Q-Score Classification	Overall Q-Score Classification	IS(B)-10[5]	IS(B)-10 Class.	Overall IS(B)-10 Class.	IS(B)-100[6]	IS(B)-100 Class.	Overall IS(B)-100 Class.	Reference
2-Methoxyethanol	109-86-4	1	100%	Liquid	99							9.7		Severe														CEC (1991)
2-Methoxyethanol	109-86-4	2	100%	Liquid	99							12.2		Severe														CEC (1991)
2-Methoxyethanol	109-86-4	3	100%	Liquid	99							12.1		Severe														CEC (1991)
2-Methoxyethanol	109-86-4	4	100%	Liquid	99							8.6		Moderate	Severe													CEC (1991)
2-Methoxyethanol	109-86-4	5	100%	Liquid	99							4.5		Slight														CEC (1991)
2-Methoxyethanol	109-86-4	6	100%	Liquid	99							0.8		Nonirritant														CEC (1991)
2-Methoxyethanol	109-86-4	7	100%	Liquid	99							3.1		Slight														CEC (1991)
2-Methoxyethanol	109-86-4	2	10%	Solution	99							7		Moderate														CEC (1991)
2-Methoxyethanol	109-86-4	3	10%	Solution	99							0		Nonirritant	Moderate													CEC (1991)
2-Methoxyethanol	109-86-4	4	10%	Solution	99							3.1		Slight														CEC (1991)
Sodium lauryl sulfate	151-21-3	1	100%	Solid	98							11.4		Severe														CEC (1991)
Sodium lauryl sulfate	151-21-3	2	100%	Solid	98							10.3		Severe														CEC (1991)
Sodium lauryl sulfate	151-21-3	3	100%	Solid	98							13.9		Severe														CEC (1991)
Sodium lauryl sulfate	151-21-3	4	100%	Solid	98							4.8		Slight	Severe													CEC (1991)
Sodium lauryl sulfate	151-21-3	6	100%	Solid	98							11.1		Severe														CEC (1991)
Sodium lauryl sulfate	151-21-3	7	100%	Solid	98							9.7		Severe														CEC (1991)
Sodium lauryl sulfate	151-21-3	2	10%	Solution	98							18.4		Severe														CEC (1991)
Sodium lauryl sulfate	151-21-3	3	10%	Solution	98							14.1		Severe	Severe													CEC (1991)
Sodium lauryl sulfate	151-21-3	4	10%	Solution	98							5.1		Moderate														CEC (1991)
Toluene	108-88-3	1	100%	Liquid	99.9							8.8		Moderate														CEC (1991)
Toluene	108-88-3	2	100%	Liquid	99.9							14.8		Severe														CEC (1991)
Toluene	108-88-3	3	100%	Liquid	99.9							15.2		Severe														CEC (1991)
Toluene	108-88-3	4	100%	Liquid	99.9							11.5		Severe	Severe													CEC (1991)
Toluene	108-88-3	5	100%	Liquid	99.9							4.6		Slight														CEC (1991)
Toluene	108-88-3	6	100%	Liquid	99.9							3.1		Slight														CEC (1991)
Toluene	108-88-3	7	100%	Liquid	99.9							4.9		Slight														CEC (1991)

Substance Name	CASRN	Lab	*In Vitro* Conc. Tested	*In Vitro* Physical Form Tested	Purity (%)	Solubility[a]	pH	IS(A)[1]	IS(A) SD	IS(A) Classification	Overall IS(A) Classification	IS(B)[2]	IS(B) SD	IS(B) Classification	Overall IS(B) Classification	S-Score[3]	S-Score Classification	Overall S-Score Classification	Q-Score[4]	Q-Score Classification	Overall Q-Score Classification	IS(B)-10[5]	IS(B)-10 Class.	Overall IS(B)-10 Class.	IS(B)-100[6]	IS(B)-100 Class.	Overall IS(B)-100 Class.	Reference
Triacetin	102-76-1	1	100%	Liquid	99							3.6		Slight														CEC (1991)
Triacetin	102-76-1	2	100%	Liquid	99							4.3		Slight														CEC (1991)
Triacetin	102-76-1	3	100%	Liquid	99							5.5		Moderate														CEC (1991)
Triacetin	102-76-1	4	100%	Liquid	99							4.4		Slight	Slight													CEC (1991)
Triacetin	102-76-1	5	100%	Liquid	99							3.3		Slight														CEC (1991)
Triacetin	102-76-1	6	100%	Liquid	99							4.3		Slight														CEC (1991)
Triacetin	102-76-1	7	100%	Liquid	99							3.1		Slight														CEC (1991)
Triacetin	102-76-1	2	10%	Solution	99							13.6		Severe														CEC (1991)
Triacetin	102-76-1	3	10%	Solution	99							2		Slight	Slight													CEC (1991)
Triacetin	102-76-1	4	10%	Solution	99							3.3		Slight														CEC (1991)
Tributyltin chloride	1461-22-9	1	100%	Solid	96							6.7		Moderate														CEC (1991)
Tributyltin chloride	1461-22-9	2	100%	Solid	96							8.9		Moderate														CEC (1991)
Tributyltin chloride	1461-22-9	3	100%	Solid	96							13.7		Severe														CEC (1991)
Tributyltin chloride	1461-22-9	4	100%	Solid	96							8.8		Moderate	Moderate													CEC (1991)
Tributyltin chloride	1461-22-9	5	100%	Solid	96							7.4		Moderate														CEC (1991)
Tributyltin chloride	1461-22-9	6	100%	Solid	96							7.9		Moderate														CEC (1991)
Tributyltin chloride	1461-22-9	7	100%	Solid	96							6.6		Moderate														CEC (1991)
Tributyltin chloride	1461-22-9	2	10%	Solution	96							15.6		Severe														CEC (1991)
Tributyltin chloride	1461-22-9	3	10%	Solution	96							9.6		Severe	Severe													CEC (1991)
Tributyltin chloride	1461-22-9	4	10%	Solution	96							11.2		Severe														CEC (1991)
Triethanolamine	102-71-6	1	100%	Liquid	97							8.6		Moderate														CEC (1991)
Triethanolamine	102-71-6	2	100%	Liquid	97							10.4		Severe														CEC (1991)
Triethanolamine	102-71-6	3	100%	Liquid	97							11.9		Severe														CEC (1991)
Triethanolamine	102-71-6	4	100%	Liquid	97							4.2		Slight	Severe													CEC (1991)
Triethanolamine	102-71-6	5	100%	Liquid	97							0		Nonirritant														CEC (1991)
Triethanolamine	102-71-6	6	100%	Liquid	97							3.7		Slight														CEC (1991)
Triethanolamine	102-71-6	7	100%	Liquid	97							7.5		Moderate														CEC (1991)

Substance Name	CASRN	Lab	*In Vitro* Conc. Tested	*In Vitro* Physical Form Tested	Purity (%)	Solubility[a]	pH	IS(A)[1]	IS(A) SD	IS(A) Classification	Overall IS(A) Classification	IS(B)[2]	IS(B) SD	IS(B) Classification	Overall IS(B) Classification	S-Score[3]	S-Score Classification	Overall S-Score Classification	Q-Score[4]	Q-Score Classification	Overall Q-Score Classification	IS(B)-10[5]	IS(B)-10 Class.	Overall IS(B)-10 Class.	IS(B)-100[6]	IS(B)-100 Class.	Overall IS(B)-100 Class.	Reference
Triethanolamine	102-71-6	2	10%	Solution	97							11.3		Severe														CEC (1991)
Triethanolamine	102-71-6	3	10%	Solution	97							2.8		Slight	Slight													CEC (1991)
Triethanolamine	102-71-6	4	10%	Solution	97							1.1		Slight														CEC (1991)
Hydroalcoholic Formulation 1-5% Alcohol Containing Formulation (PROD-00187)			100%	Solution	n.a.							4.6		Slight														Gettings et al. (1991)
Hydroalcoholic Formulation 2-10% Alcohol Containing Formulation (PROD-00183)			100%	Solution	n.a.							5		Moderate														Gettings et al. (1991)
Hydroalcoholic Formulation 3-15% Alcohol Containing Formulation (PROD-00186)			100%	Solution	n.a.							8.5		Moderate														Gettings et al. (1991)
Hydroalcoholic Formulation 4-20% Alcohol Containing Formulation (PROD-00185)			100%	Solution	n.a.							5.3		Moderate														Gettings et al. (1991)
Hydroalcoholic Formulation 5-33% Alcohol Containing Formulation (PROD-00184)			100%	Solution	n.a.																							Gettings et al. (1991)
Hydroalcoholic Formulation 6-40% Alcohol Containing Formulation (PROD-00189)			100%	Solution	n.a.							11.9		Severe														Gettings et al. (1991)
Hydroalcoholic Formulation 7-55% Alcohol Containing Formulation (PROD-00188)			100%	Solution	n.a.							12.8		Severe														Gettings et al. (1991)
Hydroalcoholic Formulation 8-65% Alcohol Containing Formulation (PROD-00180)			100%	Solution	n.a.							12.7		Severe														Gettings et al. (1991)
Hydroalcoholic Formulation 9-83% Alcohol Containing Formulation (PROD-00181)			100%	Solution	n.a.							13.8		Severe														Gettings et al. (1991)
Hydroalcoholic Formulation 10-90% Alcohol Containing Formulation (PROD-00182)			100%	Solution	n.a.							13.6		Severe														Gettings et al. (1991)
Oil/Water Emulsion-HZA			100%	Solution	n.a.			0		Nonirritant	Nonirritant	1		Slight														Gettings et al. (1994)
Oil/Water Emulsion-HZC			100%	Solution	n.a.			0.283		Nonirritant	Nonirritant	3		Slight														Gettings et al. (1994)
Oil/Water Emulsion-HZE			100%	Solution	n.a.			0.533		Nonirritant	Nonirritant	3.67		Slight														Gettings et al. (1994)
Oil/Water Emulsion-HZF			100%	Solution	n.a.			7.33		Moderate	Moderate	3.67		Slight														Gettings et al. (1994)

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Oil/Water Emulsion-HZH[a]			100%	Solution	n.a.			17.8		Severe	Severe	23		Severe														Gettings et al. (1994)
Oil/Water Emulsion-HZI			100%	Solution	n.a.			1.97		Slight	Slight	0.333		Nonirritant														Gettings et al. (1994)
Oil/Water Emulsion-HZJ			100%	Solution	n.a.			0.917		Nonirritant	Nonirritant	3		Slight														Gettings et al. (1994)
Oil/Water Emulsion-HZL			100%	Solution	n.a.			4.83		Slight	Slight	10.3		Severe														Gettings et al. (1994)
Oil/Water Emulsion-HZM			100%	Solution	n.a.			8.33		Moderate	Moderate	14.3		Severe														Gettings et al. (1994)
Oil/Water Emulsion-HZN			100%	Solution	n.a.			3.33		Slight	Slight	3.67		Slight														Gettings et al. (1994)
Oil/Water Emulsion-HZO			100%	Solution	n.a.			0.5		Nonirritant	Nonirritant	0		Nonirritant														Gettings et al. (1994)
Oil/Water Emulsion-HZR			100%	Solution	n.a.			10.6		Severe	Severe	16.3		Severe														Gettings et al. (1994)
Oil/Water Emulsion-HZS			100%	Solution	n.a.			11.6		Severe	Severe	8.33		Moderate														Gettings et al. (1994)
Oil/Water Emulsion-HZT			100%	Solution	n.a.			4.1		Slight	Slight	1		Slight														Gettings et al. (1994)
Oil/Water Emulsion-HZU			100%	Solution	n.a.			0		Nonirritant	Nonirritant	1		Slight														Gettings et al. (1994)
Oil/Water Emulsion-HZV			100%	Solution	n.a.			0.6		Nonirritant	Nonirritant	0		Nonirritant														Gettings et al. (1994)
Oil/Water Emulsion-HZW			100%	Solution	n.a.			0.167		Nonirritant	Nonirritant	5		Moderate														Gettings et al. (1994)
Oil/Water Emulsion-HZY			100%	Solution	n.a.			17		Severe	Severe	9.67		Severe														Gettings et al. (1994)
Surfactant Based Formulation 1-HZA			10%	Solution	n.a.			7.8		Moderate	Moderate	9.6		Severe														Gettings et al. (1996)
Surfactant Based Formulation 2-HZB			10%	Solution	n.a.			4.8		Slight	Slight	7.3		Moderate														Gettings et al. (1996)
Surfactant Based Formulation 3-HZC			10%	Solution	n.a.			9.5		Severe	Severe	15.3		Severe														Gettings et al. (1996)
Surfactant Based Formulation 4-HZD			10%	Solution	n.a.			5.2		Moderate	Moderate	8.7		Moderate														Gettings et al. (1996)
Surfactant Based Formulation 5-HZE			10%	Solution	n.a.			3.8		Slight	Slight	11.4		Severe														Gettings et al. (1996)
Surfactant Based Formulation 6-HZF			10%	Solution	n.a.			8.3		Moderate	Moderate	10.9		Severe														Gettings et al. (1996)
Surfactant Based Formulation 7-HZG			10%	Solution	n.a.			6.3		Moderate	Moderate	7.1		Moderate														Gettings et al. (1996)
Surfactant Based Formulation 8-HZH			10%	Solution	n.a.			1.3		Slight	Slight	3.5		Slight														Gettings et al. (1996)
Surfactant Based Formulation 9-HZI			10%	Solution	n.a.			9.3		Severe	Severe	15.2		Severe														Gettings et al. (1996)
Surfactant Based Formulation 10-HZJ			10%	Solution	n.a.			2.2		Slight	Slight	6.2		Moderate														Gettings et al. (1996)
Surfactant Based Formulation 11-HZK			10%	Solution	n.a.			8.8		Moderate	Moderate	9.4		Severe														Gettings et al. (1996)
Surfactant Based Formulation 12-HZL			10%	Solution	n.a.			9.6		Severe	Severe	12.4		Severe														Gettings et al. (1996)
Surfactant Based Formulation 13-HZM			10%	Solution	n.a.			4.1		Slight	Slight	2.7		Slight														Gettings et al. (1996)

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Surfactant Based Formulation 14-HZN			10%	Solution	n.a.			6.1		Moderate	Moderate	8		Moderate														Gettings et al. (1996)
Surfactant Based Formulation 15-HZP			10%	Solution	n.a.			4.7		Slight	Slight	4.4		Slight														Gettings et al. (1996)
Surfactant Based Formulation 16-HZQ			10%	Solution	n.a.			4.9		Slight	Slight	4.2		Slight														Gettings et al. (1996)
Surfactant Based Formulation 17-HZR			10%	Solution	n.a.			7.7		Moderate	Moderate	5.3		Moderate														Gettings et al. (1996)
Surfactant Based Formulation 18-HZS			10%	Solution	n.a.			8.8		Moderate	Moderate	12.2		Severe														Gettings et al. (1996)
Surfactant Based Formulation 19-HZT			10%	Solution	n.a.			0.2		Nonirritant	Nonirritant	3.5		Slight														Gettings et al. (1996)
Surfactant Based Formulation 20-HZU			10%	Solution	n.a.			3.7		Slight	Slight	6.2		Moderate														Gettings et al. (1996)
Surfactant Based Formulation 21-HZV			10%	Solution	n.a.			7.7		Moderate	Moderate	8.7		Moderate														Gettings et al. (1996)
Surfactant Based Formulation 22-HZW			10%	Solution	n.a.			7.8		Moderate	Moderate	5.1		Moderate														Gettings et al. (1996)
Surfactant Based Formulation 23-HZX			10%	Solution	n.a.			9		Severe	Severe	11.3		Severe														Gettings et al. (1996)
Surfactant Based Formulation 24-HZY			10%	Solution	n.a.			8.7		Moderate	Moderate	11.7		Severe														Gettings et al. (1996)
Surfactant Based Formulation 25-HZZ			10%	Solution	n.a.			0.7		Nonirritant	Nonirritant	1.1		Slight														Gettings et al. (1996)
Allyl alcohol	107-18-6		100%	Liquid	n.p.							12.4	2.3	Severe														Gilleron et al. (1996)
2-Aminophemol	95-55-6		100%	Solid	n.p.							0.8	0.7	Nonirritant														Gilleron et al. (1996)
Anthracene	120-12-7		100%	Solid	n.p.							0	0	Nonirritant														Gilleron et al. (1996)
Benzethonium chloride	121-54-0		100%	Solid	n.p.							15.4	3.1	Severe														Gilleron et al. (1996)
Gamma-butyrolactone	96-48-0		100%	Liquid	n.p.							13.9	1.8	Severe														Gilleron et al. (1996)
Cyclohexanone	108-94-1		100%	Liquid	n.p.							14.5	3.8	Severe														Gilleron et al. (1996)
Deoxycholic acid, sodium salt	302-95-4		100%	Solid	n.p.							9.7	5.8	Severe														Gilleron et al. (1996)
Diacetone alcohol	123-42-2		100%	Liquid	n.p.							15.1	2.7	Severe														Gilleron et al. (1996)
Dibenzoyl-L-tartaric acid	2743-38-6		100%	Solid	n.p.							4.2	2.5	Slight														Gilleron et al. (1996)
2,4-Dicholor-5-sulfamolyl-benzoic acid	2736-23-4		100%	Solid	n.p.							3.8	2.2	Slight														Gilleron et al. (1996)
Dimethyl biguanidine	657-24-9		100%	Solid	n.p.							8.4	2.2	Moderate														Gilleron et al. (1996)
Dimethyl sulfoxide	67-68-5		100%	Liquid	n.p.							11.3	3.7	Severe														Gilleron et al. (1996)
EDTA dipotassium	25105-12-9		100%	Solid	n.p.							0	0	Nonirritant														Gilleron et al. (1996)
Ethanol	64-17-5		100%	Liquid	n.p.							11.3	2.8	Severe														Gilleron et al. (1996)
2-Ethoxyethanol	110-80-5		100%	Liquid	n.p.							10.5	2.7	Severe														Gilleron et al. (1996)

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Ethylacetoacetate	141-97-9		100%	Liquid	n.p.							10	3.2	Severe														Gilleron et al. (1996)
Furan	110-00-9		100%	Liquid	n.p.							5.5	1	Moderate														Gilleron et al. (1996)
Gluconolactone	90-80-2		100%	Solid	n.p.							4.6	3.2	Slight														Gilleron et al. (1996)
DL-Glutamic acid	19285-83-7		100%	Solid	n.p.							0.7	1.2	Nonirritant														Gilleron et al. (1996)
3-Glycidopropyltrimethoxysilane	2530-83-8		100%	Liquid	n.p.							4.3	1	Slight														Gilleron et al. (1996)
Hexadecyltrimethylammonium bromide	57-09-0		100%	Liquid	n.p.							10.8	4.8	Severe														Gilleron et al. (1996)
Hexane	110-54-3		100%	Liquid	n.p.							3.1	2.7	Slight														Gilleron et al. (1996)
Imidazole	288-32-4		100%	Solid	n.p.							18.7	0.9	Severe														Gilleron et al. (1996)
Iminodibenzyl	94-19-9		100%	Solid	n.p.							0	0	Nonirritant														Gilleron et al. (1996)
N-Lauroylsarcosine, sodium salt	7631-98-3		100%	Solid	n.p.							12.7	4.3	Severe														Gilleron et al. (1996)
Laurylsulfobetaine	14933-08-5		100%	Unknown	n.p.							8.3	1.2	Moderate														Gilleron et al. (1996)
Magnesium carbonate	56378-72-4		100%	Solid	n.p.							1.4	1.9	Slight														Gilleron et al. (1996)
Methanol	67-56-1		100%	Liquid	n.p.							12.2	3.3	Severe														Gilleron et al. (1996)
2-Methoxyethanol	109-86-4		100%	Liquid	n.p.							14.5	0.7	Severe														Gilleron et al. (1996)
Methyl isobutyl ketone	108-10-1		100%	Liquid	n.p.							10.5	1.5	Severe														Gilleron et al. (1996)
MYRJ 45			100%	Unknown	n.p.							0.00	0.00	Nonirritant														Gilleron et al. (1996)
1-Nitropropane	108-03-2		100%	Liquid	n.p.							2.8	2.7	Slight														Gilleron et al. (1996)
Octanol	111-87-5		100%	Liquid	n.p.							9.8	1.7	Severe														Gilleron et al. (1996)
2,4-Pentadione	123-54-6		100%	Liquid	n.p.							8.8	3	Moderate														Gilleron et al. (1996)
1-Phenyl-3-pyrazolidine	92-43-3		100%	Solid	n.p.							0.5	0.4	Nonirritant														Gilleron et al. (1996)
Polyoxyethylene 23 lauryl ether			100%	Solid	n.p.							1.5	2.6	Slight														Gilleron et al. (1996)
Promethazine HCl	58-33-3		100%	Solid	n.p.							13.9	2.1	Severe														Gilleron et al. (1996)
Propyl-4-hydroxybenzoate	94-13-3		100%	Solid	n.p.							1.9	1	Slight														Gilleron et al. (1996)
Pyridine	110-86-1		100%	Liquid	n.p.							15.8	3.6	Severe														Gilleron et al. (1996)
Quinacrine	69-05-6		100%	Solid	n.p.							6.5	2.2	Moderate														Gilleron et al. (1996)
Tetraaminopyrimidine sulfate	5392-28-9		100%	Solid	n.p.							0.5	0.9	Nonirritant														Gilleron et al. (1996)
Thiourea	62-56-6		100%	Solid	n.p.							13.7	4.4	Severe														Gilleron et al. (1996)

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1,2,3-Trichloropropane	96-18-4		100%	Liquid	n.p.							7.9	1.7	Moderate														Gilleron et al. (1996)
1,2,4-Trichloropropane	95-63-6		100%	Liquid	n.p.							4.5	2.9	Slight														Gilleron et al. (1996)
Triethanolamine	102-71-6		100%	Liquid	n.p.							9.6	3.5	Severe														Gilleron et al. (1996)
Triton X-155	9010-44-0		100%	Surfactant	n.p.							3.9	2.3	Slight														Gilleron et al. (1996)
Acetone	67-64-1		100%	Liquid	>99	water soluble						15.32	0.33	Severe														Gilleron et al. (1997)
Ammonium nitrate	6484-52-2		100%	Solid	>99.9	water soluble						15.34	1.24	Severe														Gilleron et al. (1997)
L-Aspartic acid	70-47-3		100%	Solid	95	water soluble						1.06	1.2	Slight														Gilleron et al. (1997)
Benzalkonium chloride	8001-54-5		100%	Unknown	98	surfactant						14.8	0.53	Severe														Gilleron et al. (1997)
Benzalkonium chloride	8001-54-5		100%	Unknown	98	surfactant						15.05	0.27	Severe														Gilleron et al. (1997)
Benzalkonium chloride	8001-54-5		100%	Unknown	98	surfactant						15.14	0.25	Severe														Gilleron et al. (1997)
Benzoyl-L-tartaric acid	2743-38-6		100%	Solid	n.p.	water soluble						13.34	4.24	Severe														Gilleron et al. (1997)
Butyl acetate	123-86-4		100%	Liquid	99	water insoluble						17.21	1.84	Severe														Gilleron et al. (1997)
Gamma-butyrolactone	96-48-0		100%	Liquid	>99	water soluble						19.39	0.83	Severe														Gilleron et al. (1997)
Captan 90 concentrate	133-06-2		100%	Solid	90	water soluble						15.07	0.27	Severe														Gilleron et al. (1997)
4-Carboxybenzaldehyde	619-66-9		100%	Solid	95	water insoluble						3.95	4.69	Slight														Gilleron et al. (1997)
Cetylpyridinium bromide	140-72-7		100%	Solid	98	surfactant						12.68	1.52	Severe														Gilleron et al. (1997)
Cetylpyridinium bromide	140-72-7		100%	Solid	98	surfactant						13.53	2.42	Severe														Gilleron et al. (1997)
Cetylpyridinium bromide	140-72-7		100%	Solid	98	surfactant						14.6	0.43	Severe														Gilleron et al. (1997)
Chlorhexidine	55-56-1		100%	Solid	99.5	water insoluble						14.87	3.78	Severe														Gilleron et al. (1997)
Cyclohexanol	108-93-0		100%	Liquid	97	water soluble						18.96	0.1	Severe														Gilleron et al. (1997)
Dibenzyl phosphate	1623-08-1		100%	Solid	99.5	water insoluble						15.16	0.47	Severe														Gilleron et al. (1997)
2,6-Dichlorobenzoyl chloride	4659-45-4		100%	Liquid	99	water insoluble						10.74	1.74	Severe														Gilleron et al. (1997)
2,2-Dimethylbutanoic acid	595-37-9		100%	Liquid	>99	water insoluble						15.31	0.24	Severe														Gilleron et al. (1997)
2,5-Dimethylhexanediol	110-03-2		100%	Solid	99.5	water insoluble						15.33	0.38	Severe														Gilleron et al. (1997)
Ethanol	64-17-5		100%	Liquid	n.p.	water soluble						14.97	0.04	Severe														Gilleron et al. (1997)
Ethyl acetate	141-78-6		100%	Liquid	99	water soluble						19.32	0.06	Severe														Gilleron et al. (1997)
2-Ethyl-1-hexanol	104-76-7		100%	Liquid	99	water soluble						12.71	2.96	Severe														Gilleron et al. (1997)

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Ethyl-2-methylacetoacetate	609-14-3		100%	Liquid	ca. 97	water insoluble						12.94	2.94	Severe														Gilleron et al. (1997)
Ethyl trimethyl acetate	3938-95-2		100%	Liquid	99	water insoluble						13.82	2.73	Severe														Gilleron et al. (1997)
Fomesafen	72128-02-0		100%	Solid	97.5	water soluble						1.21	1.29	Slight														Gilleron et al. (1997)
Glycerol	56-81-5		100%	Liquid	99.5	water soluble						14.78	0.75	Severe														Gilleron et al. (1997)
Hexanol	111-27-3		100%	Liquid	98	water insoluble						17.56	0.4	Severe														Gilleron et al. (1997)
Imidazole	288-32-4		100%	Solid	99	water soluble						19.43	0.49	Severe														Gilleron et al. (1997)
Isobutanol	78-83-1		100%	Liquid	99.9	water insoluble						19.41	0.08	Severe														Gilleron et al. (1997)
Isopropanol	67-63-0		100%	Liquid	99.9	water soluble						14.8	0.21	Severe														Gilleron et al. (1997)
Maneb	12427-38-2		100%	Solid	90	water soluble						0.16	0.24	Nonirritant														Gilleron et al. (1997)
Methyl acetate	79-20-9		100%	Liquid	98	water soluble						18.98	0.75	Severe														Gilleron et al. (1997)
Methyl cyanoacetate	105-34-0		100%	Liquid	99	water soluble						16.31	1.23	Severe														Gilleron et al. (1997)
Methylcyclopentane	96-37-7		100%	Liquid	>99	water insoluble						17.14	1.63	Severe														Gilleron et al. (1997)
Methyl ethyl ketone	78-93-3		100%	Liquid	99	water soluble						18.35	2.52	Severe														Gilleron et al. (1997)
Methyl isobutyl ketone	108-10-1		100%	Liquid	98	water insoluble						17.75	2.2	Severe														Gilleron et al. (1997)
1-Naphthalene acetic acid	86-87-3		100%	Solid	99	water soluble						7.46	2.37	Moderate														Gilleron et al. (1997)
1-Naphthalene acetic acid, Na salt	61-31-4		100%	Solid	95	water soluble						15.16	0.49	Severe														Gilleron et al. (1997)
Octanol	111-87-5		100%	Liquid	>99	water insoluble						16.7	0.81	Severe														Gilleron et al. (1997)
Parafluoraniline	371-40-4		100%	Liquid	99	water insoluble						15.49	1.63	Severe														Gilleron et al. (1997)
Polyethylene glycol 400	25322-68-3		100%	Liquid	n.p.	surfactant						14.68	0.55	Severe														Gilleron et al. (1997)
Potassium cyanate	590-28-3		100%	Solid	97	water soluble						14.27	1.15	Severe														Gilleron et al. (1997)
Promethazine HCl	58-33-3		100%	Solid	98	water soluble						6.27	1.41	Moderate														Gilleron et al. (1997)
Pyridine	110-86-1		100%	Liquid	>99	water soluble						17.79	2.44	Severe														Gilleron et al. (1997)
Quinacrine	69-05-6		100%	Solid	n.p.	water soluble						7.29	0.6	Moderate														Gilleron et al. (1997)
Sodium hydroxide	1310-73-2		100%	Solid	n.p.	water soluble						19.01	0.13	Severe														Gilleron et al. (1997)
Sodium hydroxide	1310-73-2		100%	Solid	n.p.	water soluble						20.56	0.08	Severe														Gilleron et al. (1997)
Sodium lauryl sulfate	151-21-3		100%	Solid	98	surfactant						12.38	1.82	Severe														Gilleron et al. (1997)
Sodium lauryl sulfate	151-21-3		100%	Solid	98	surfactant						15.05	0.29	Severe														Gilleron et al. (1997)

Substance Name	CASRN	Lab	*In Vitro* Conc. Tested	*In Vitro* Physical Form Tested	Purity (%)	Solubility[a]	pH	IS(A)[1]	IS(A) SD	IS(A) Classification	Overall IS(A) Classification	IS(B)[2]	IS(B) SD	IS(B) Classification	Overall IS(B) Classification	S-Score[3]	S-Score Classification	Overall S-Score Classification	Q-Score[4]	Q-Score Classification	Overall Q-Score Classification	IS(B)-10[5]	IS(B)-10 Class.	Overall IS(B)-10 Class.	IS(B)-100[6]	IS(B)-100 Class.	Overall IS(B)-100 Class.	Reference
Sodium oxalate	62-76-0		100%	Solid	>99	water soluble						14.2	0.71	Severe														Gilleron et al. (1997)
Sodium perborate	10486-00-7		100%	Solid	98.6	water soluble						13.19	1.78	Severe														Gilleron et al. (1997)
Tetraaminopyrimidine sulfate	5392-28-9		100%	Solid	97	water insoluble						4.33	0.23	Slight														Gilleron et al. (1997)
Thiourea	62-56-6		100%	Solid	>99	water soluble						17.89	1.53	Severe														Gilleron et al. (1997)
Toluene	108-88-3		100%	Liquid	99	water soluble						16.09	1.62	Severe														Gilleron et al. (1997)
Trichloroacetic acid	76-03-9		100%	Liquid	n.p.	water soluble						15.7	0.11	Severe														Gilleron et al. (1997)
Trichloroacetic acid	76-03-9		100%	Liquid	n.p.	water soluble						15.72	0.15	Severe														Gilleron et al. (1997)
Triton X-100	9002-93-1		100%	Liquid	98	surfactant						10.94	0.8	Severe														Gilleron et al. (1997)
Triton X-100	9002-93-1		100%	Liquid	98	surfactant						13.73	0.48	Severe														Gilleron et al. (1997)
Tween 20	9005-64-5		100%	Liquid	98	surfactant						14.47	0.36	Severe														Gilleron et al. (1997)
Acetic acid	64-19-7	1	10%	Solution	n.p.		2.4	16.5	2.89	Severe																		Hagino et al. (1999)/Submitted Y. Ohno Data
Acetic acid	64-19-7	2	10%	Solution	n.p.		2.4	16	3.92	Severe																		Hagino et al. (1999)/Submitted Y. Ohno Data
Acetic acid	64-19-7	3	10%	Solution	n.p.		2.4	17.25	6.24	Severe	Severe																	Hagino et al. (1999)/Submitted Y. Ohno Data
Acetic acid	64-19-7	4	10%	Solution	n.p.		2.4	19.5	1.91	Severe																		Hagino et al. (1999)/Submitted Y. Ohno Data
Acetic acid	64-19-7	5	10%	Solution	n.p.		2.4	17.5	4.04	Severe																		Hagino et al. (1999)/Submitted Y. Ohno Data
Butanol	71-36-3	1	10%	Suspension	n.p.		7.31	8.25	2.87	Moderate																		Hagino et al. (1999)/Submitted Y. Ohno Data
Butanol	71-36-3	2	10%	Suspension	n.p.		7.31	10.5	1.91	Severe																		Hagino et al. (1999)/Submitted Y. Ohno Data
Butanol	71-36-3	3	10%	Suspension	n.p.		7.31	12	0.00	Severe	Severe																	Hagino et al. (1999)/Submitted Y. Ohno Data
Butanol	71-36-3	4	10%	Suspension	n.p.		7.31	12	0.00	Severe																		Hagino et al. (1999)/Submitted Y. Ohno Data
Butanol	71-36-3	5	10%	Suspension	n.p.		7.31	5.75	1.50	Moderate																		Hagino et al. (1999)/Submitted Y. Ohno Data

Substance Name	CASRN	Lab	*In Vitro* Conc. Tested	*In Vitro* Physical Form Tested	Purity (%)	Solubility[a]	pH	IS(A)[1]	IS(A) SD	IS(A) Classification	Overall IS(A) Classification	IS(B)[2]	IS(B) SD	IS(B) Classification	Overall IS(B) Classification	S-Score[3]	S-Score Classification	Overall S-Score Classification	Q-Score[4]	Q-Score Classification	Overall Q-Score Classification	IS(B)-10[5]	IS(B)-10 Class.	Overall IS(B)-10 Class.	IS(B)-100[6]	IS(B)-100 Class.	Overall IS(B)-100 Class.	Reference
Cetyltrimethylammonium bromide	57-09-0	1	10%	Solution	n.p.		5.89	19	1.63	Severe																		Hagino et al. (1999)/Submitted Y. Ohno Data
Cetyltrimethylammonium bromide	57-09-0	2	10%	Solution	n.p.		5.89	13.25	2.22	Severe																		Hagino et al. (1999)/Submitted Y. Ohno Data
Cetyltrimethylammonium bromide	57-09-0	3	10%	Solution	n.p.		5.89	18.5	1.91	Severe	Severe																	Hagino et al. (1999)/Submitted Y. Ohno Data
Cetyltrimethylammonium bromide	57-09-0	4	10%	Solution	n.p.		5.89	11	2.45	Severe																		Hagino et al. (1999)/Submitted Y. Ohno Data
Cetyltrimethylammonium bromide	57-09-0	5	10%	Solution	n.p.		5.89	9	0.00	Severe																		Hagino et al. (1999)/Submitted Y. Ohno Data
Chlorhexidine gluconate solution (20% solution)	18472-51-0	1	10%	Solution	n.p.		6.56	19	1.63	Severe																		Hagino et al. (1999)/Submitted Y. Ohno Data
Chlorhexidine gluconate solution (20% solution)	18472-51-0	2	10%	Solution	n.p.		6.56	13.5	1.00	Severe																		Hagino et al. (1999)/Submitted Y. Ohno Data
Chlorhexidine gluconate solution (20% solution)	18472-51-0	3	10%	Solution	n.p.		6.56	16	2.45	Severe	Severe																	Hagino et al. (1999)/Submitted Y. Ohno Data
Chlorhexidine gluconate solution (20% solution)	18472-51-0	4	10%	Solution	n.p.		6.56	11.75	4.86	Severe																		Hagino et al. (1999)/Submitted Y. Ohno Data
Chlorhexidine gluconate solution (20% solution)	18472-51-0	5	10%	Solution	n.p.		6.56	9	0.00	Severe																		Hagino et al. (1999)/Submitted Y. Ohno Data
Di(2-ethylhexyl) sodium sulfosuccinate	577-11-7	1	10%	Suspension	n.p.		6.54	10	0.00	Severe																		Hagino et al. (1999)/Submitted Y. Ohno Data
Di(2-ethylhexyl) sodium sulfosuccinate	577-11-7	2	10%	Suspension	n.p.		6.54	10	1.63	Severe																		Hagino et al. (1999)/Submitted Y. Ohno Data
Di(2-ethylhexyl) sodium sulfosuccinate	577-11-7	3	10%	Suspension	n.p.		6.54	10.25	3.50	Severe	Severe																	Hagino et al. (1999)/Submitted Y. Ohno Data
Di(2-ethylhexyl) sodium sulfosuccinate	577-11-7	4	10%	Suspension	n.p.		6.54	12	0.00	Severe																		Hagino et al. (1999)/Submitted Y. Ohno Data
Di(2-ethylhexyl) sodium sulfosuccinate	577-11-7	5	10%	Suspension	n.p.		6.54	5	0.00	Moderate																		Hagino et al. (1999)/Submitted Y. Ohno Data
Diisopropanolamine	110-97-4	1	10%	Solution	n.p.		11.89	8.25	2.36	Moderate																		Hagino et al. (1999)/Submitted Y. Ohno Data
Diisopropanolamine	110-97-4	2	10%	Solution	n.p.		11.89	8.5	4.04	Moderate																		Hagino et al. (1999)/Submitted Y. Ohno Data
Diisopropanolamine	110-97-4	3	10%	Solution	n.p.		11.89	9	1.15	Severe	Moderate																	Hagino et al. (1999)/Submitted Y. Ohno Data
Diisopropanolamine	110-97-4	4	10%	Solution	n.p.		11.89	12	0.00	Severe																		Hagino et al. (1999)/Submitted Y. Ohno Data
Diisopropanolamine	110-97-4	5	10%	Solution	n.p.		11.89	5	0.00	Moderate																		Hagino et al. (1999)/Submitted Y. Ohno Data

Substance Name	CASRN	Lab	*In Vitro* Conc. Tested	*In Vitro* Physical Form Tested	Purity (%)	Solubility[a]	pH	IS(A)[1]	IS(A) SD	IS(A) Classification	Overall IS(A) Classification	IS(B)[2]	IS(B) SD	IS(B) Classification	Overall IS(B) Classification	S-Score[3]	S-Score Classification	Overall S-Score Classification	Q-Score[4]	Q-Score Classification	Overall Q-Score Classification	IS(B)-10[5]	IS(B)-10 Class.	Overall IS(B)-10 Class.	IS(B)-100[6]	IS(B)-100 Class.	Overall IS(B)-100 Class.	Reference
Domiphen bromide	538-71-6	1	10%	Solution	n.p.		6.22	19	0.00	Severe																		Hagino et al. (1999)/Submitted Y. Ohno Data
Domiphen bromide	538-71-6	2	10%	Solution	n.p.		6.22	15.25	2.36	Severe																		Hagino et al. (1999)/Submitted Y. Ohno Data
Domiphen bromide	538-71-6	3	10%	Solution	n.p.		6.22	14.75	1.50	Severe	Severe																	Hagino et al. (1999)/Submitted Y. Ohno Data
Domiphen bromide	538-71-6	4	10%	Solution	n.p.		6.22	12.25	2.36	Severe																		Hagino et al. (1999)/Submitted Y. Ohno Data
Domiphen bromide	538-71-6	5	10%	Solution	n.p.		6.22	9	1.22	Severe																		Hagino et al. (1999)/Submitted Y. Ohno Data
Ethanol	64-17-5	1	10%	Solution	n.p.		5.9	0	0.00	Nonirritant																		Hagino et al. (1999)/Submitted Y. Ohno Data
Ethanol	64-17-5	2	10%	Solution	n.p.		5.9	1.25	2.50	Slight																		Hagino et al. (1999)/Submitted Y. Ohno Data
Ethanol	64-17-5	3	10%	Solution	n.p.		5.9	10.5	1.91	Severe	Slight																	Hagino et al. (1999)/Submitted Y. Ohno Data
Ethanol	64-17-5	4	10%	Solution	n.p.		5.9	1.5	1.73	Slight																		Hagino et al. (1999)/Submitted Y. Ohno Data
Ethanol	64-17-5	5	10%	Solution	n.p.		5.9	1.25	2.50	Slight																		Hagino et al. (1999)/Submitted Y. Ohno Data
Ethanol	64-17-5	1	100%	Liquid	n.p.			18.75	3.30	Severe																		Hagino et al. (1999)/Submitted Y. Ohno Data
Ethanol	64-17-5	2	100%	Liquid	n.p.			16	2.45	Severe																		Hagino et al. (1999)/Submitted Y. Ohno Data
Ethanol	64-17-5	3	100%	Liquid	n.p.			11.5	1.00	Severe	Severe																	Hagino et al. (1999)/Submitted Y. Ohno Data
Ethanol	64-17-5	4	100%	Liquid	n.p.			17	0.00	Severe																		Hagino et al. (1999)/Submitted Y. Ohno Data
Ethanol	64-17-5	5	100%	Liquid	n.p.			10.5	1.73	Severe																		Hagino et al. (1999)/Submitted Y. Ohno Data
Glycolic acid	79-14-1	1	10%	Solution	n.p.		1.76	19.5	1.00	Severe																		Hagino et al. (1999)/Submitted Y. Ohno Data
Glycolic acid	79-14-1	2	10%	Solution	n.p.		1.76	20	1.15	Severe																		Hagino et al. (1999)/Submitted Y. Ohno Data
Glycolic acid	79-14-1	3	10%	Solution	n.p.		1.76	17.75	3.95	Severe	Severe																	Hagino et al. (1999)/Submitted Y. Ohno Data
Glycolic acid	79-14-1	4	10%	Solution	n.p.		1.76	12.25	2.36	Severe																		Hagino et al. (1999)/Submitted Y. Ohno Data
Glycolic acid	79-14-1	5	10%	Solution	n.p.		1.76	12.75	2.50	Severe																		Hagino et al. (1999)/Submitted Y. Ohno Data

Substance Name	CASRN	Lab	*In Vitro* Conc. Tested	*In Vitro* Physical Form Tested	Purity (%)	Solubility[a]	pH	IS(A)[1]	IS(A) SD	IS(A) Classification	Overall IS(A) Classification	IS(B)[2]	IS(B) SD	IS(B) Classification	Overall IS(B) Classification	S-Score[3]	S-Score Classification	Overall S-Score Classification	Q-Score[4]	Q-Score Classification	Overall Q-Score Classification	IS(B)-10[5]	IS(B)-10 Class.	Overall IS(B)-10 Class.	IS(B)-100[6]	IS(B)-100 Class.	Overall IS(B)-100 Class.	Reference
Lactic acid	50-21-5	1	10%	Solution	n.p.		1.94	20.5	1.00	Severe																		Hagino et al. (1999)/Submitted Y. Ohno Data
Lactic acid	50-21-5	2	10%	Solution	n.p.		1.94	14.25	2.06	Severe																		Hagino et al. (1999)/Submitted Y. Ohno Data
Lactic acid	50-21-5	3	10%	Solution	n.p.		1.94	19.5	1.91	Severe	Severe																	Hagino et al. (1999)/Submitted Y. Ohno Data
Lactic acid	50-21-5	4	10%	Solution	n.p.		1.94	18.5	1.91	Severe																		Hagino et al. (1999)/Submitted Y. Ohno Data
Lactic acid	50-21-5	5	10%	Solution	n.p.		1.94	10.25	2.50	Severe																		Hagino et al. (1999)/Submitted Y. Ohno Data
Lactic acid	50-21-5	1	100%	Liquid	n.p.			21	0.00	Severe																		Hagino et al. (1999)/Submitted Y. Ohno Data
Lactic acid	50-21-5	2	100%	Liquid	n.p.			6.25	2.50	Moderate																		Hagino et al. (1999)/Submitted Y. Ohno Data
Lactic acid	50-21-5	3	100%	Liquid	n.p.			16	1.15	Severe	Severe																	Hagino et al. (1999)/Submitted Y. Ohno Data
Lactic acid	50-21-5	4	100%	Liquid	n.p.			15.25	2.50	Severe																		Hagino et al. (1999)/Submitted Y. Ohno Data
Lactic acid	50-21-5	5	100%	Liquid	n.p.			11.5	2.89	Severe																		Hagino et al. (1999)/Submitted Y. Ohno Data
Monoethanolamine	141-43-5	1	10%	Solution	n.p.		12.58	12	0.00	Severe																		Hagino et al. (1999)/Submitted Y. Ohno Data
Monoethanolamine	141-43-5	2	10%	Solution	n.p.		12.58	12	0.00	Severe																		Hagino et al. (1999)/Submitted Y. Ohno Data
Monoethanolamine	141-43-5	3	10%	Solution	n.p.		12.58	12	0.00	Severe	Severe																	Hagino et al. (1999)/Submitted Y. Ohno Data
Monoethanolamine	141-43-5	4	10%	Solution	n.p.		12.58	12	0.00	Severe																		Hagino et al. (1999)/Submitted Y. Ohno Data
Monoethanolamine	141-43-5	5	10%	Solution	n.p.		12.58	12	0.00	Severe																		Hagino et al. (1999)/Submitted Y. Ohno Data
Potassium laurate	10124-65-9	1	10%	Solution	n.p.		10.49	20	1.15	Severe																		Hagino et al. (1999)/Submitted Y. Ohno Data
Potassium laurate	10124-65-9	2	10%	Solution	n.p.		10.49	13.25	2.50	Severe																		Hagino et al. (1999)/Submitted Y. Ohno Data
Potassium laurate	10124-65-9	3	10%	Solution	n.p.		10.49	12	0.00	Severe	Severe																	Hagino et al. (1999)/Submitted Y. Ohno Data
Potassium laurate	10124-65-9	4	10%	Solution	n.p.		10.49	12	0.00	Severe																		Hagino et al. (1999)/Submitted Y. Ohno Data
Potassium laurate	10124-65-9	5	10%	Solution	n.p.		10.49	19.33	0.82	Severe																		Hagino et al. (1999)/Submitted Y. Ohno Data

Substance Name	CASRN	Lab	*In Vitro* Conc. Tested	*In Vitro* Physical Form Tested	Purity (%)	Solubility[a]	pH	IS(A)[1]	IS(A) SD	IS(A) Classification	Overall IS(A) Classification	IS(B)[2]	IS(B) SD	IS(B) Classification	Overall IS(B) Classification	S-Score[3]	S-Score Classification	Overall S-Score Classification	Q-Score[4]	Q-Score Classification	Overall Q-Score Classification	IS(B)-10[5]	IS(B)-10 Class.	Overall IS(B)-10 Class.	IS(B)-100[6]	IS(B)-100 Class.	Overall IS(B)-100 Class.	Reference
Stearyltrimethylammonium chloride	15461-40-2	1	10%	Solution	n.p.		4.24	16.75	2.06	Severe																		Hagino et al. (1999)/Submitted Y. Ohno Data
Stearyltrimethylammonium chloride	15461-40-2	2	10%	Solution	n.p.		4.24	13	2.00	Severe																		Hagino et al. (1999)/Submitted Y. Ohno Data
Stearyltrimethylammonium chloride	15461-40-2	3	10%	Solution	n.p.		4.24	15.75	3.50	Severe	Severe																	Hagino et al. (1999)/Submitted Y. Ohno Data
Stearyltrimethylammonium chloride	15461-40-2	4	10%	Solution	n.p.		4.24	13.5	1.00	Severe																		Hagino et al. (1999)/Submitted Y. Ohno Data
Stearyltrimethylammonium chloride	15461-40-2	5	10%	Solution	n.p.		4.24	9	0.00	Severe																		Hagino et al. (1999)/Submitted Y. Ohno Data
Triethanolamine	102-71-6	1	10%	Solution	n.p.		11.26	1.5	2.38	Slight																		Hagino et al. (1999)/Submitted Y. Ohno Data
Triethanolamine	102-71-6	2	10%	Solution	n.p.		11.26	3.75	4.79	Slight																		Hagino et al. (1999)/Submitted Y. Ohno Data
Triethanolamine	102-71-6	3	10%	Solution	n.p.		11.26	11	1.15	Severe	Slight																	Hagino et al. (1999)/Submitted Y. Ohno Data
Triethanolamine	102-71-6	4	10%	Solution	n.p.		11.26	6	1.63	Moderate																		Hagino et al. (1999)/Submitted Y. Ohno Data
Triethanolamine	102-71-6	5	10%	Solution	n.p.		11.26	2.5	2.89	Slight																		Hagino et al. (1999)/Submitted Y. Ohno Data
Triethanolamine	102-71-6	1	100%	Liquid	n.p.			5	0.00	Moderate																		Hagino et al. (1999)/Submitted Y. Ohno Data
Triethanolamine	102-71-6	2	100%	Liquid	n.p.			6.75	3.50	Moderate																		Hagino et al. (1999)/Submitted Y. Ohno Data
Triethanolamine	102-71-6	3	100%	Liquid	n.p.			11.5	1.00	Severe	Moderate																	Hagino et al. (1999)/Submitted Y. Ohno Data
Triethanolamine	102-71-6	4	100%	Liquid	n.p.			12	0.00	Severe																		Hagino et al. (1999)/Submitted Y. Ohno Data
Triethanolamine	102-71-6	5	100%	Liquid	n.p.			6.75	3.50	Moderate																		Hagino et al. (1999)/Submitted Y. Ohno Data
Ethanol	64-17-5		10%	Solution	n.p.		7.2	4		Slight	Slight																	Kojima et al. (1995)
Potassium laurate	10124-65-9		10%	Solution	98		9.4	14.3		Severe	Severe																	Kojima et al. (1995)
Sodium lauryl sulfate	151-21-3		10%	Solution	98		5.4	7.5		Moderate	Moderate																	Kojima et al. (1995)
Stearyltrimethylammonium chloride	15461-40-2		10%	Solution	65		5.5	19.3		Severe	Severe																	Kojima et al. (1995)
Triton X-100	9002-93-1		10%	Solution	n.p.		5.75	5		Moderate	Moderate																	Kojima et al. (1995)
7-Acetoxyheptanal[7]		MD	100%, 10%, and ITC	-	n.p.	insoluble	n.s.															3.1	Slight	Slight	4.9	Slight	Severe	Spielmann et al. (1996)
7-Acetoxyheptanal		WA	100%, 10%, and ITC	-	n.p.	insoluble	n.s.															0	Nonirritant		17	Severe		Spielmann et al. (1996)
n-Acetyl-Methionine	1115-47-5	MD	100%, 10%, and ITC	-	n.p.	83	2.2															13.6	Severe	Severe	n.p.		Severe	Spielmann et al. (1996)

Substance Name	CASRN	Lab	*In Vitro* Conc. Tested	*In Vitro* Physical Form Tested	Purity (%)	Solubility[a]	pH	IS(A)[1]	IS(A) SD	IS(A) Classification	Overall IS(A) Classification	IS(B)[2]	IS(B) SD	IS(B) Classification	Overall IS(B) Classification	S-Score[3]	S-Score Classification	Overall S-Score Classification	Q-Score[4]	Q-Score Classification	Overall Q-Score Classification	IS(B)-10[5]	IS(B)-10 Class.	Overall IS(B)-10 Class.	IS(B)-100[6]	IS(B)-100 Class.	Overall IS(B)-100 Class.	Reference
n-Acetyl-Methionine	1115-47-5	WA	100%, 10%, and ITC	-	n.p.	83	2.2															6.1	Moderate	Severe	10.6	Severe	Severe	Spielmann et al. (1996)
Ambuphylline	5634-34-4	BG	100%, 10%, and ITC	-	n.p.	600	9															10.7	Severe	Severe	12.8	Severe	Severe	Spielmann et al. (1996)
Ambuphylline	5634-34-4	MD	100%, 10%, and ITC	-	n.p.	600	9															15.8	Severe		16.9	Severe		Spielmann et al. (1996)
4-Amino-5-methoxy-2-methylbenzenesulfonic acid	6471-78-9	AP	100%, 10%, and ITC	-	n.p.	3	1.5															14.8	Severe	Moderate	14.4	Severe	Severe	Spielmann et al. (1996)
4-Amino-5-methoxy-2-methylbenzenesulfonic acid	6471-78-9	WA	100%, 10%, and ITC	-	n.p.	3	1.5															7	Moderate		13.6	Severe		Spielmann et al. (1996)
4-Amino-5-methoxy-2-methylbenzenesulfonic acid	6471-78-9	BG	100%, 10%, and ITC	-	n.p.	3	1.5															7.6	Moderate		8.5	Moderate		Spielmann et al. (1996)
Ammonium persulfate	7727-54-0	HO	100%, 10%, and ITC	-	n.p.	560	1.5															4.4	Slight	Slight	n.p.			Spielmann et al. (1996)
Ammonium persulfate	7727-54-0	WA	100%, 10%, and ITC	-	n.p.	560	1.5															n.p.			n.p.			Spielmann et al. (1996)
Anisole	100-66-3	AP	100%, 10%, and ITC	-	n.p.	insoluble	n.s.															7.3	Moderate	Moderate	19.1	Severe	Severe	Spielmann et al. (1996)
Anisole	100-66-3	HK	100%, 10%, and ITC	-	n.p.	insoluble	n.s.															0	Nonirritant		18.5	Severe		Spielmann et al. (1996)
B 25		BG	100%, 10%, and ITC	-	n.p.	insoluble	n.s.															0	Nonirritant	Nonirritant	0	Nonirritant	Nonirritant	Spielmann et al. (1996)
B 25		WA	100%, 10%, and ITC	-	n.p.	insoluble	n.s.															0	Nonirritant		0	Nonirritant		Spielmann et al. (1996)
n-Butanal	123-72-8	HK	100%, 10%, and ITC	-	n.p.	71	<7															1.2	Slight	Moderate	20.3	Severe	Severe	Spielmann et al. (1996)
n-Butanal	123-72-8	HO	100%, 10%, and ITC	-	n.p.	71	<7															6.7	Moderate		18.1	Severe		Spielmann et al. (1996)
n-Butanol	71-36-3	BD	100%, 10%, and ITC	-	n.p.	79	7															9.6	Severe	Severe	13	Severe	Severe	Spielmann et al. (1996)
n-Butanol	71-36-3	HK	100%, 10%, and ITC	-	n.p.	79	7															18.3	Severe		20.2	Severe		Spielmann et al. (1996)
Butyl carbamate	592-35-8	BD	100%, 10%, and ITC	-	n.p.	1	n.s.															0	Nonirritant	Severe	11.5	Severe	Severe	Spielmann et al. (1996)
Butyl carbamate	592-35-8	MD	100%, 10%, and ITC	-	n.p.	1	n.s.															10.9	Severe		11.6	Severe		Spielmann et al. (1996)
Butyl carbamate	592-35-8	BG	100%, 10%, and ITC	-	n.p.	1	n.s.															9.5	Severe		14.9	Severe		Spielmann et al. (1996)

Substance Name	CASRN	Lab	*In Vitro* Conc. Tested	*In Vitro* Physical Form Tested	Purity (%)	Solubility[a]	pH	IS(A)[1]	IS(A) SD	IS(A) Classification	Overall IS(A) Classification	IS(B)[2]	IS(B) SD	IS(B) Classification	Overall IS(B) Classification	S-Score[3]	S-Score Classification	Overall S-Score Classification	Q-Score[4]	Q-Score Classification	Overall Q-Score Classification	IS(B)-10[5]	IS(B)-10 Class.	Overall IS(B)-10 Class.	IS(B)-100[6]	IS(B)-100 Class.	Overall IS(B)-100 Class.	Reference
Caffeine sodium benzoate	8000-95-1	BD	100%, 10%, and ITC	-	n.p.	500	7															4.6	Slight	Moderate	7.4	Moderate	Severe	Spielmann et al. (1996)
Caffeine sodium benzoate	8000-95-1	WA	100%, 10%, and ITC	-	n.p.	500	7															7.9	Moderate		17.9	Severe		Spielmann et al. (1996)
Caffeine sodium benzoate	8000-95-1	BG	100%, 10%, and ITC	-	n.p.	500	7															6.6	Moderate		14	Severe		Spielmann et al. (1996)
Caffeine sodium salicylate	8002-85-5	BG	100%, 10%, and ITC	-	n.p.	400	7															7.4	Moderate	Severe	16	Severe	Severe	Spielmann et al. (1996)
Caffeine sodium salicylate	8002-85-5	WA	100%, 10%, and ITC	-	n.p.	400	7															9.8	Severe		18.8	Severe		Spielmann et al. (1996)
Camphen	79-92-5	BG	100%, 10%, and ITC	-	n.p.	insoluble	7															2	Severe	Severe	4	Slight	Slight	Spielmann et al. (1996)
Camphen	79-92-5	HK	100%, 10%, and ITC	-	n.p.	insoluble	7															10	Severe		n.p.			Spielmann et al. (1996)
Cerium-2-ethylhexanoate	24593-34-8	BG	100%, 10%, and ITC	-	n.p.		3															6.9	Moderate	Moderate	15.1	Severe	Severe	Spielmann et al. (1996)
Cerium-2-ethylhexanoate	24593-34-8	WA	100%, 10%, and ITC	-	n.p.		3															7.9	Moderate		19.25	Severe		Spielmann et al. (1996)
1-Chloroctane-8-ol		AP	100%, 10%, and ITC	-	n.p.	insoluble	n.s.															6.8	Moderate	Moderate	18.7	Severe	Severe	Spielmann et al. (1996)
1-Chloroctane-8-ol		MD	100%, 10%, and ITC	-	n.p.	insoluble	n.s.															4.3	Slight		14.3	Severe		Spielmann et al. (1996)
3-Cyclohexene-1-methanol	1679-51-2	BG	100%, 10%, and ITC	-	n.p.	insoluble	n.s.															10.1	Severe	Severe	18.9	Severe	Severe	Spielmann et al. (1996)
3-Cyclohexene-1-methanol	1679-51-2	HO	100%, 10%, and ITC	-	n.p.	insoluble	n.s.															11.8	Severe		19	Severe		Spielmann et al. (1996)
DC 8		BG	100%, 10%, and ITC	-	n.p.	insoluble	n.s.															0	Nonirritant	Nonirritant	0	Nonirritant	Moderate	Spielmann et al. (1996)
DC 8		WA	100%, 10%, and ITC	-	n.p.	insoluble	n.s.															0	Nonirritant		5	Moderate		Spielmann et al. (1996)
1,4-Dibutoxy-benzene	104-36-9	HO	100%, 10%, and ITC	-	n.p.	0.2	7															4.2	Slight	Slight	0	Nonirritant	Nonirritant	Spielmann et al. (1996)
1,4-Dibutoxy-benzene	104-36-9	WA	100%, 10%, and ITC	-	n.p.	0.2	7															0	Nonirritant		n.p.			Spielmann et al. (1996)
Diepoxid 126	2386-87-0	AP	100%, 10%, and ITC	-	n.p.	insoluble	n.s.															6	Moderate	Moderate	10	Severe	Severe	Spielmann et al. (1996)
Diepoxid 126	2386-87-0	MD	100%, 10%, and ITC	-	n.p.	insoluble	n.s.															8.6	Moderate		15.6	Severe		Spielmann et al. (1996)
Diepoxid 126	2386-87-0	BG	100%, 10%, and ITC	-	n.p.	insoluble	n.s.															1.9	Slight		6	Moderate		Spielmann et al. (1996)

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2,5-Dimethylhexanediol	110-03-2	HK	100%, 10%, and ITC	-	n.p.		n.s.															9.2	Severe	Severe	16.6	Severe	Severe	Spielmann et al. (1996)
2,5-Dimethylhexanediol	110-03-2	HO	100%, 10%, and ITC	-	n.p.		n.s.															4.1	Slight		11.1	Severe		Spielmann et al. (1996)
2,5-Dimethylhexanediol	110-03-2	BG	100%, 10%, and ITC	-	n.p.		n.s.																					Spielmann et al. (1996)
3,6-Dimethyloctanol		BG	100%, 10%, and ITC	-	n.p.	poorly soluble	7															0.3	Nonirritant	Nonirritant	4.3	Slight	Slight	Spielmann et al. (1996)
3,6-Dimethyloctanol		BD	100%, 10%, and ITC	-	n.p.	poorly soluble	7															0	Nonirritant		4.3	Slight		Spielmann et al. (1996)
4,4-Dimethyl-3-oxo-pentanenitrile	59997-51-2	AP	100%, 10%, and ITC	-	n.p.	0.6	n.s.															4.3	Slight	Moderate	6.7	Moderate	Moderate	Spielmann et al. (1996)
4,4-Dimethyl-3-oxo-pentanenitrile	59997-51-2	WA	100%, 10%, and ITC	-	n.p.	0.6	n.s.															5.6	Moderate		5.7	Moderate		Spielmann et al. (1996)
1-(2,6-dimethylphenoxy)-2-propanone	53012-41-2	HK	100%, 10%, and ITC	-	n.p.	insoluble	5															18.9	Severe	Severe	19.3	Severe	Severe	Spielmann et al. (1996)
1-(2,6-dimethylphenoxy)-2-propanone	53012-41-2	WA	100%, 10%, and ITC	-	n.p.	insoluble	5															2.6	Slight		12	Severe		Spielmann et al. (1996)
1-(2,6-dimethylphenoxy)-2-propanone	53012-41-2	BG	100%, 10%, and ITC	-	n.p.	insoluble	5															0.75	Nonirritant		4.1	Slight		Spielmann et al. (1996)
Diphocars		HK	100%, 10%, and ITC	-	n.p.	soluble	n.s.															18.3	Severe	Severe	17.9	Severe	Severe	Spielmann et al. (1996)
Diphocars		HO	100%, 10%, and ITC	-	n.p.	soluble	n.s.															11.1	Severe		12.3	Severe		Spielmann et al. (1996)
1,2-Dodecanediol	1119-87-5	AP	100%, 10%, and ITC	-	n.p.	insoluble	n.s.															12.1	Severe	Slight	2.3	Slight	Slight	Spielmann et al. (1996)
1,2-Dodecanediol	1119-87-5	BG	100%, 10%, and ITC	-	n.p.	insoluble	n.s.															1.8	Slight		4.1	Slight		Spielmann et al. (1996)
1,2-Dodecanediol	1119-87-5	BG	100%, 10%, and ITC	-	n.p.	insoluble	n.s.															2.54	Slight			Nonirritant		Spielmann et al. (1996)
DTPA Pentasodium salt	140-01-2	BG	100%, 10%, and ITC	-	n.p.	readily soluble	11.5															15.66	Severe	Severe	19.4	Severe	Severe	Spielmann et al. (1996)
DTPA Pentasodium salt	140-01-2	WA	100%, 10%, and ITC	-	n.p.	readily soluble	11.5															15.5	Severe		19.9	Severe		Spielmann et al. (1996)
Ede 140		WA	100%, 10%, and ITC	-	n.p.	insoluble	n.s.															0	Nonirritant	Slight	0	Nonirritant	Slight	Spielmann et al. (1996)
Ede 140		BD	100%, 10%, and ITC	-	n.p.	insoluble	n.s.															3.4	Slight		4.6	Slight		Spielmann et al. (1996)
1,2-Epoxycyclooctane	286-62-4	MD	100%, 10%, and ITC	-	n.p.	<2.5	4.5															n.p.		Severe	n.p.		Moderate	Spielmann et al. (1996)
1,2-Epoxycyclooctane	286-62-4	AP	100%, 10%, and ITC	-	n.p.	<2.5	4.5															3.1	Slight		7	Moderate		Spielmann et al. (1996)
1,2-Epoxydodecane	2855-19-8	MD	100%, 10%, and ITC	-	n.p.	insoluble	n.s.															0	Nonirritant	Slight	1.4	Slight	Moderate	Spielmann et al. (1996)

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1,2-Epoxydodecane	2855-19-8	HO	100%, 10%, and ITC	-	n.p.	insoluble	n.s.															4.1	Slight	Slight	8.5	Moderate	Moderate	Spielmann et al. (1996)
Ethiosan		AP	100%, 10%, and ITC	-	n.p.	5	8.5															3.8	Slight	Slight	n.p.			Spielmann et al. (1996)
Ethiosan		WA	100%, 10%, and ITC	-	n.p.	5	8.5															0	Nonirritant		n.p.			Spielmann et al. (1996)
Ethyl butanal	97-96-1	HO	100%, 10%, and ITC	-	n.p.	10	<7															3.6	Slight	Slight	17.4	Severe	Severe	Spielmann et al. (1996)
Ethyl butanal	97-96-1	WA	100%, 10%, and ITC	-	n.p.	10	<7															0	Nonirritant		18.7	Severe		Spielmann et al. (1996)
Gadopentetic acid dimeglumine salt	86050-77-3	WA	100%, 10%, and ITC	-	n.p.	soluble	n.s.															6.4	Severe	Severe	8.2	Moderate	Moderate	Spielmann et al. (1996)
Gadopentetic acid dimeglumine salt	86050-77-3	BG	100%, 10%, and ITC	-	n.p.	soluble	n.s.															3	Severe		3.2	Slight		Spielmann et al. (1996)
Genomoll	115-96-8	HO	100%, 10%, and ITC	-	n.p.	5	6															9.2	Severe	Severe	11.6	Severe	Severe	Spielmann et al. (1996)
Genomoll	115-96-8	WA	100%, 10%, and ITC	-	n.p.	5	6															9.4	Severe		9.9	Severe		Spielmann et al. (1996)
C12/C14-Glucoside		BD	100%, 10%, and ITC	-	n.p.	readily soluble	9															8.4	Moderate	Severe	16.7	Severe	Severe	Spielmann et al. (1996)
C12/C14-Glucoside		HK	100%, 10%, and ITC	-	n.p.	readily soluble	9															10.1	Severe		16.3	Severe		Spielmann et al. (1996)
C12/C14-Glucoside		BG	100%, 10%, and ITC	-	n.p.	readily soluble	9															10.2	Severe		16.5	Severe		Spielmann et al. (1996)
L-Glutamic acid hydrochloride	138-15-8	HO	100%, 10%, and ITC	-	n.p.	490	0.9															14.2	Severe	Severe	11.7	Severe	Severe	Spielmann et al. (1996)
L-Glutamic acid hydrochloride	138-15-8	MD	100%, 10%, and ITC	-	n.p.	490	0.9															11.7	Severe		15.2	Severe		Spielmann et al. (1996)
Glycediol		MD	100%, 10%, and ITC	-	n.p.	insoluble	n.s.															0	Nonirritant	Slight	0.58	Nonirritant	Slight	Spielmann et al. (1996)
Glycediol		HO	100%, 10%, and ITC	-	n.p.	insoluble	n.s.															1.8	Slight		3.5	Slight		Spielmann et al. (1996)
Granuform	30525-89-4	BD	100%, 10%, and ITC	-	n.p.	250	4															2.9	Slight	Slight	0	Nonirritant	Nonirritant	Spielmann et al. (1996)
Granuform	30525-89-4	HO	100%, 10%, and ITC	-	n.p.	250	4															0	Nonirritant		0	Nonirritant		Spielmann et al. (1996)
Hexahydrofarnesylacetone	502-69-2	BG	100%, 10%, and ITC	-	n.p.	poorly soluble	n.s.															2.3	Slight	Slight	8	Moderate	Moderate	Spielmann et al. (1996)
Hexahydrofarnesylacetone	502-69-2	BD	100%, 10%, and ITC	-	n.p.	poorly soluble	n.s.															1.2	Slight		4.2	Slight		Spielmann et al. (1996)
Hexamethylenetetramine	100-97-0	WA	100%, 10%, and ITC	-	n.p.	874	8.5															5.8	Moderate	Moderate	11.1	Severe	Severe	Spielmann et al. (1996)
Hexamethylenetetramine	100-97-0	MD	100%, 10%, and ITC	-	n.p.	874	8.5															4.3	Slight		11.2	Severe		Spielmann et al. (1996)

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1,2,6-Hexanetriol	106-69-4	HK	100%, 10%, and ITC	-	n.p.		4.5															11.5	Severe	Severe	18.8	Severe	Severe	Spielmann et al. (1996)
1,2,6-Hexanetriol	106-69-4	HO	100%, 10%, and ITC	-	n.p.		4.5															4.3	Slight		15.3	Severe		Spielmann et al. (1996)
Hnol		AP	100%, 10%, and ITC	-	n.p.	insoluble	n.s.															0.8	Nonirritant	Nonirritant	2.1	Slight	Moderate	Spielmann et al. (1996)
Hnol		WA	100%, 10%, and ITC	-	n.p.	insoluble	n.s.															0	Nonirritant		6	Moderate		Spielmann et al. (1996)
Hoe MBF		BD	100%, 10%, and ITC	-	n.p.	100	4.3															0	Nonirritant	Nonirritant	0	Nonirritant	Nonirritant	Spielmann et al. (1996)
Hoe MBF		MD	100%, 10%, and ITC	-	n.p.	100	4.3															0	Nonirritant		0.35	Nonirritant		Spielmann et al. (1996)
Hydo 98		BD	100%, 10%, and ITC	-	n.p.	soluble	6.5															10.4	Severe	Severe	11.2	Severe	Severe	Spielmann et al. (1996)
Hydo 98		MD	100%, 10%, and ITC	-	n.p.	soluble	6.5															12.9	Severe		n.p.			Spielmann et al. (1996)
2-Hydroxyethyl imino disodium acetate	135-37-5	AP	100%, 10%, and ITC	-	n.p.		10.6															13.4	Severe	Severe	15.5	Severe	Severe	Spielmann et al. (1996)
2-Hydroxyethyl imino disodium acetate	135-37-5	HO	100%, 10%, and ITC	-	n.p.		10.6															8.9	Moderate		11	Severe		Spielmann et al. (1996)
2-Hydroxyisobutyric acid	594-61-6	BD	100%, 10%, and ITC	-	n.p.	1900	1															10.8	Severe	Severe	11.3	Severe	Severe	Spielmann et al. (1996)
2-Hydroxyisobutyric acid	594-61-6	WA	100%, 10%, and ITC	-	n.p.	1900	1															14.9	Severe		15.6	Severe		Spielmann et al. (1996)
Hypo 20		BG	100%, 10%, and ITC	-	n.p.	readily soluble	6.5															7.2	Moderate	Moderate	8.9	Moderate	Moderate	Spielmann et al. (1996)
Hypo 20		HO	100%, 10%, and ITC	-	n.p.	readily soluble	6.5															0	Nonirritant		4.12	Slight		Spielmann et al. (1996)
Hypo 36		AP	100%, 10%, and ITC	-	n.p.	readily soluble	7															4	Severe	Severe	15.9	Severe	Severe	Spielmann et al. (1996)
Hypo 36		WA	100%, 10%, and ITC	-	n.p.	readily soluble	7															4.2	Severe		10	Severe		Spielmann et al. (1996)
Hypo 45		BD	100%, 10%, and ITC	-	n.p.	readily soluble	7															11.1	Severe	Slight	4.4	Slight	Severe	Spielmann et al. (1996)
Hypo 45		WA	100%, 10%, and ITC	-	n.p.	readily soluble	7															2.5	Slight		8.7	Moderate		Spielmann et al. (1996)
Hypo 45		BG	100%, 10%, and ITC	-	n.p.	readily soluble	7															1.9	Slight		11.9	Severe		Spielmann et al. (1996)
Hypo 54		BG	100%, 10%, and ITC	-	n.p.	soluble	6.5															4.3	Slight	Slight	4.1	Slight	Slight	Spielmann et al. (1996)
Hypo 54		HO	100%, 10%, and ITC	-	n.p.	soluble	6.5															4	Slight		4.2	Slight		Spielmann et al. (1996)
Hyton		AP	100%, 10%, and ITC	-	n.p.	soluble	8.5															17	Severe	Severe	18.6	Severe	Severe	Spielmann et al. (1996)

Substance Name	CASRN	Lab	*In Vitro* Conc. Tested	*In Vitro* Physical Form Tested	Purity (%)	Solubility*	pH	IS(A)[1]	IS(A) SD	IS(A) Classification	Overall IS(A) Classification	IS(B)[2]	IS(B) SD	IS(B) Classification	Overall IS(B) Classification	S-Score[3]	S-Score Classification	Overall S-Score Classification	Q-Score[4]	Q-Score Classification	Overall Q-Score Classification	IS(B)-10[5]	IS(B)-10 Class.	Overall IS(B)-10 Class.	IS(B)-100[6]	IS(B)-100 Class.	Overall IS(B)-100 Class.	Reference
Hyton		BG	100%, 10%, and ITC	-	n.p.	soluble	8.5															13.5	Severe	Severe	18.2	Severe	Severe	Spielmann et al. (1996)
Iminodiacetic acid	142-73-4	AP	100%, 10%, and ITC	-	n.p.	42	2.3															15.6	Severe	Severe	12.8	Severe	Severe	Spielmann et al. (1996)
Iminodiacetic acid	142-73-4	BD	100%, 10%, and ITC	-	n.p.	42	2.3															0.75	Nonirritant		0.85	Nonirritant		Spielmann et al. (1996)
Iminodiacetic acid	142-73-4	BG	100%, 10%, and ITC	-	n.p.	42	2.3															8.4	Moderate		6.9	Moderate		Spielmann et al. (1996)
Isobornyl acetate	125-12-2	HO	100%, 10%, and ITC	-	n.p.	< 1	n.s.															4.1	Slight	Slight	4.6	Slight	Moderate	Spielmann et al. (1996)
Isobornyl acetate	125-12-2	BD	100%, 10%, and ITC	-	n.p.	< 1	n.s.															1.7	Slight		8.1	Moderate		Spielmann et al. (1996)
Isobutanal	78-84-2	WA	100%, 10%, and ITC	-	n.p.	67	<7															2.1	Slight	Slight	19.4	Severe	Severe	Spielmann et al. (1996)
Isobutanal	78-84-2	HK	100%, 10%, and ITC	-	n.p.	67	<7															0	Nonirritant		20	Severe		Spielmann et al. (1996)
Isodecylglucoside		AP	100%, 10%, and ITC	-	n.p.	readily soluble	9															17.2	Severe	Severe	18	Severe	Severe	Spielmann et al. (1996)
Isodecylglucoside		HO	100%, 10%, and ITC	-	n.p.	readily soluble	9															9.9	Severe		10.7	Severe		Spielmann et al. (1996)
Isononylaldehyde	35127-50-5	BG	100%, 10%, and ITC	-	n.p.	0.1	<7															0	Nonirritant	Nonirritant	4.5	Slight	Severe	Spielmann et al. (1996)
Isononylaldehyde	35127-50-5	WA	100%, 10%, and ITC	-	n.p.	0.1	<7															0	Nonirritant		10	Severe		Spielmann et al. (1996)
alpha-Ketoglutaric acid	328-50-7	AP	100%, 10%, and ITC	-	n.p.	1000	1.75															19.1	Severe	Severe	19.8	Severe	Severe	Spielmann et al. (1996)
alpha-Ketoglutaric acid	328-50-7	BG	100%, 10%, and ITC	-	n.p.	1000	1.75															18.8	Severe		19.7	Severe		Spielmann et al. (1996)
Lactic acid	79-33-4	PhI	100%, 10%, and ITC	-	n.p.	readily soluble	2															17.6	Severe	Severe	19.6	Severe	Severe	Spielmann et al. (1996)
alpha-Lactid	4511-42-6	AP	100%, 10%, and ITC	-	n.p.	soluble	3															13.5	Severe	Severe	4	Slight	Slight	Spielmann et al. (1996)
alpha-Lactid	4511-42-6	BG	100%, 10%, and ITC	-	n.p.	soluble	3															1.8	Slight		1.1	Slight		Spielmann et al. (1996)
alpha-Lactid	4511-42-6	BG	100%, 10%, and ITC	-	n.p.	soluble	3															10.5	Severe		6.6	Moderate		Spielmann et al. (1996)
L-Lysine Monohydrate	39665-12-8	BD	100%, 10%, and ITC	-	n.p.	1500	10															10	Severe	Severe	10.4	Severe	Severe	Spielmann et al. (1996)
L-Lysine Monohydrate	39665-12-8	HO	100%, 10%, and ITC	-	n.p.	1500	10															8.25	Moderate		16.9	Severe		Spielmann et al. (1996)
Mecre		HK	100%, 10%, and ITC	-	n.p.	mixable	7															n.p.			n.p.			Spielmann et al. (1996)
Mecre		MD	100%, 10%, and ITC	-	n.p.	mixable	7															n.p.			n.p.			Spielmann et al. (1996)
3-Mercapto-1,2,4-triazole	3179-31-5	HK	100%, 10%, and ITC	-	n.p.	85	4															18.3	Severe	Severe	n.p.			Spielmann et al. (1996)
3-Mercapto-1,2,4-triazole	3179-31-5	MD	100%, 10%, and ITC	-	n.p.	85	4															4.3	Slight		n.p.			Spielmann et al. (1996)
m-Methoxybenzaldehyde	591-31-1	MD	100%, 10%, and ITC	-	n.p.	poorly soluble	n.s.															4.1	Slight	Slight	13.7	Severe	Severe	Spielmann et al. (1996)
m-Methoxybenzaldehyde	591-31-1	BD	100%, 10%, and ITC	-	n.p.	poorly soluble	n.s.															2.2	Slight		11.6	Severe		Spielmann et al. (1996)

Substance Name	CASRN	Lab	*In Vitro* Conc. Tested	*In Vitro* Physical Form Tested	Purity (%)	Solubility[a]	pH	IS(A)[1]	IS(A) SD	IS(A) Classification	Overall IS(A) Classification	IS(B)[2]	IS(B) SD	IS(B) Classification	Overall IS(B) Classification	S-Score[3]	S-Score Classification	Overall S-Score Classification	Q-Score[4]	Q-Score Classification	Overall Q-Score Classification	IS(B)-10[5]	IS(B)-10 Class.	Overall IS(B)-10 Class.	IS(B)-100[6]	IS(B)-100 Class.	Overall IS(B)-100 Class.	Reference
Methyl acetate	79-20-9	BD	100%, 10%, and ITC	-	n.p.	250	7															4.4	Slight	Slight	19.8	Severe	Severe	Spielmann et al. (1996)
Methyl acetate	79-20-9	HO	100%, 10%, and ITC	-	n.p.	250	7															4.3	Slight		16.1	Severe		Spielmann et al. (1996)
Methylpentynol	77-75-8	AP	100%, 10%, and ITC	-	n.p.	soluble	n.s.															15.4	Severe	Severe	20.1	Severe	Severe	Spielmann et al. (1996)
Methylpentynol	77-75-8	BD	100%, 10%, and ITC	-	n.p.	soluble	n.s.															12.3	Severe		12.9	Severe		Spielmann et al. (1996)
N-(2-methylphenyl)-Imidodi-carbonimidic diamide	93-69-6	AP	100%, 10%, and ITC	-	n.p.	40	11.5															17.1	Severe	Severe	4.7	Slight	Slight	Spielmann et al. (1996)
N-(2-methylphenyl)-Imidodi-carbonimidic diamide	93-69-6	MD	100%, 10%, and ITC	-	n.p.	40	11.5															17.7	Severe		n.p.			Spielmann et al. (1996)
2-Methyl-1-propanol	78-83-1	HK	100%, 10%, and ITC	-	n.p.	15	3															17.7	Severe	Severe	20.4	Severe	Severe	Spielmann et al. (1996)
2-Methyl-1-propanol	78-83-1	MD	100%, 10%, and ITC	-	n.p.	15	3															17.9	Severe		19.2	Severe		Spielmann et al. (1996)
Methyltriglycol	112-35-6	BD	100%, 10%, and ITC	-	n.p.	readily soluble	7															4.9	Slight	Severe	12.5	Severe	Severe	Spielmann et al. (1996)
Methyltriglycol	112-35-6	HO	100%, 10%, and ITC	-	n.p.	readily soluble	7															4.1	Severe		17	Severe		Spielmann et al. (1996)
Methyltriglycol	112-35-6	AP	100%, 10%, and ITC	-	n.p.	readily soluble	7															11	Severe	Severe	20.4	Severe	Severe	Spielmann et al. (1996)
Methyltriglycol	112-35-6	HO	100%, 10%, and ITC	-	n.p.	readily soluble	7															3	Severe		12.8	Severe		Spielmann et al. (1996)
Napt		HO	100%, 10%, and ITC	-	n.p.	1000	n.s.															4.3	Slight	Slight	10.3	Severe	Severe	Spielmann et al. (1996)
Napt		WA	100%, 10%, and ITC	-	n.p.	1000	n.s.															1.9	Slight		5.7	Moderate		Spielmann et al. (1996)
Nitro-bis-octylamide		BG	100%, 10%, and ITC	-	n.p.	insoluble	n.s.															1.7	Slight	Slight	6.5	Moderate	Moderate	Spielmann et al. (1996)
Nitro-bis-octylamide		HK	100%, 10%, and ITC	-	n.p.	insoluble	n.s.															0	Nonirritant		1.6	Slight		Spielmann et al. (1996)
Olak		HK	100%, 10%, and ITC	-	n.p.	soluble	8.3															18.9	Severe	Severe	19.5	Severe	Severe	Spielmann et al. (1996)
Olak		MD	100%, 10%, and ITC	-	n.p.	soluble	8.3															16.1	Severe		17	Severe		Spielmann et al. (1996)
Ölesulf		BD	100%, 10%, and ITC	-	n.p.	soluble	8															16.9	Severe	Severe	18.9	Severe	Severe	Spielmann et al. (1996)
Ölesulf		HK	100%, 10%, and ITC	-	n.p.	soluble	8															16.8	Severe		19.6	Severe		Spielmann et al. (1996)
Phenylephrine hydrochloride	61-76-7	AP	100%, 10%, and ITC	-	n.p.	1000	7															8.6	Moderate	Severe	18.3	Severe	Severe	Spielmann et al. (1996)
Phenylephrine hydrochloride	61-76-7	HK	100%, 10%, and ITC	-	n.p.	1000	7															11.1	Severe		19.9	Severe		Spielmann et al. (1996)

Substance Name	CASRN	Lab	*In Vitro* Conc. Tested	*In Vitro* Physical Form Tested	Purity (%)	Solubility*	pH	IS(A)[1]	IS(A) SD	IS(A) Classification	Overall IS(A) Classification	IS(B)[2]	IS(B) SD	IS(B) Classification	Overall IS(B) Classification	S-Score[3]	S-Score Classification	Overall S-Score Classification	Q-Score[4]	Q-Score Classification	Overall Q-Score Classification	IS(B)-10[5]	IS(B)-10 Class.	Overall IS(B)-10 Class.	IS(B)-100[6]	IS(B)-100 Class.	Overall IS(B)-100 Class.	Reference
Phenylthiourea	103-85-5	AP	100%, 10%, and ITC	-	n.p.	1	5.5															4	Slight	Slight	3.1	Slight	Slight	Spielmann et al. (1996)
Phenylthiourea	103-85-5	BD	100%, 10%, and ITC	-	n.p.	1	5.5															0	Nonirritant		0	Nonirritant		Spielmann et al. (1996)
Phosphonat A		AP	100%, 10%, and ITC	-	n.p.	3.6	2.1															6.8	Moderate	Moderate	3.5	Slight	Severe	Spielmann et al. (1996)
Phosphonat A		BG	100%, 10%, and ITC	-	n.p.	3.6	2.1															6.6	Moderate		10.1	Severe		Spielmann et al. (1996)
Acefyllin piperazinate	18833-13-1	HK	100%, 10%, and ITC	-	n.p.	625	5															18.5	Severe	Severe	15.3	Severe	Severe	Spielmann et al. (1996)
Acefyllin piperazinate	18833-13-1	WA	100%, 10%, and ITC	-	n.p.	625	5															0	Nonirritant		14.6	Severe		Spielmann et al. (1996)
Acefyllin piperazinate	18833-13-1	BG	100%, 10%, and ITC	-	n.p.	625	5															2.9	Slight		9	Severe		Spielmann et al. (1996)
PO 2		AP	100%, 10%, and ITC	-	n.p.	insoluble	n.s.															4.3	Slight	Slight	0.3	Nonirritant	Nonirritant	Spielmann et al. (1996)
PO 2		WA	100%, 10%, and ITC	-	n.p.	insoluble	n.s.															0	Nonirritant		0	Nonirritant		Spielmann et al. (1996)
Polyethylene glycol butyl ether	9004-77-7	AP	100%, 10%, and ITC	-	n.p.	1000	6															10.9	Severe	Severe	19.3	Severe	Severe	Spielmann et al. (1996)
Polyethylene glycol butyl ether	9004-77-7	WA	100%, 10%, and ITC	-	n.p.	1000	6															15.7	Severe		19.2	Severe		Spielmann et al. (1996)
Polyethylene glycol dimethyl ether	24991-55-7	HO	100%, 10%, and ITC	-	n.p.	readily soluble	7															4.1	Slight	Slight	7.6	Moderate	Severe	Spielmann et al. (1996)
Polyethylene glycol dimethyl ether	24991-55-7	WA	100%, 10%, and ITC	-	n.p.	readily soluble	7															0	Nonirritant		19.8	Severe		Spielmann et al. (1996)
Polyethylene glycol	25322-68-3	MD	100%, 10%, and ITC	-	n.p.	750	n.s.															1	Slight	Slight	6.6	Moderate	Moderate	Spielmann et al. (1996)
Polyethylene glycol	25322-68-3	WA	100%, 10%, and ITC	-	n.p.	750	n.s.															0	Nonirritant		7.7	Moderate		Spielmann et al. (1996)
Polyhexamethylene guanidine		BD	100%, 10%, and ITC	-	n.p.	soluble	7.1															9.2	Severe	Severe	15.5	Severe	Severe	Spielmann et al. (1996)
Polyhexamethylene guanidine		BG	100%, 10%, and ITC	-	n.p.	soluble	7.1															11	Severe		14.6	Severe		Spielmann et al. (1996)
Polysolvan	7397-62-8	AP	100%, 10%, and ITC	-	n.p.	80	7															16.5	Severe	Severe	19.4	Severe	Severe	Spielmann et al. (1996)
Polysolvan	7397-62-8	HO	100%, 10%, and ITC	-	n.p.	80	7															15.8	Severe		15.9	Severe		Spielmann et al. (1996)
Potassium cyanate	590-28-3	AP	100%, 10%, and ITC	-	n.p.	750	10															18.8	Severe	Severe	19.4	Severe	Severe	Spielmann et al. (1996)
Potassium cyanate	590-28-3	MD	100%, 10%, and ITC	-	n.p.	750	10															15.8	Severe		15.9	Severe		Spielmann et al. (1996)
Potassium hexacyanoferrate II	14459-95-1	HK	100%, 10%, and ITC	-	n.p.	250	9.5															17.8	Severe	Severe	17.2	Severe	Severe	Spielmann et al. (1996)
Potassium hexacyanoferrate II	14459-95-1	HO	100%, 10%, and ITC	-	n.p.	250	9.5															15.2	Severe		6.3	Moderate		Spielmann et al. (1996)
Potassium hexacyanoferrate III	13756-66-2	BD	100%, 10%, and ITC	-	n.p.	310	8															4.2	Slight	Moderate	5.7	Moderate	Moderate	Spielmann et al. (1996)
Potassium hexacyanoferrate III	13756-66-2	MD	100%, 10%, and ITC	-	n.p.	310	8															6.25	Moderate		6.45	Moderate		Spielmann et al. (1996)
2-Pseudojonon		HK	100%, 10%, and ITC	-	n.p.	0.1	n.s.															8.7	Moderate	Moderate	7.3	Moderate	Moderate	Spielmann et al. (1996)
2-Pseudojonon		BG	100%, 10%, and ITC	-	n.p.	0.1	n.s.															2.8	Slight		4.1	Slight		Spielmann et al. (1996)

Substance Name	CASRN	Lab	*In Vitro* Conc. Tested	*In Vitro* Physical Form Tested	Purity (%)	Solubility[a]	pH	IS(A)[1]	IS(A) SD	IS(A) Classification	Overall IS(A) Classification	IS(B)[2]	IS(B) SD	IS(B) Classification	Overall IS(B) Classification	S-Score[3]	S-Score Classification	Overall S-Score Classification	Q-Score[4]	Q-Score Classification	Overall Q-Score Classification	IS(B)-10[5]	IS(B)-10 Class.	Overall IS(B)-10 Class.	IS(B)-100[6]	IS(B)-100 Class.	Overall IS(B)-100 Class.	Reference
RK Blau		HK	100%, 10%, and ITC	-	n.p.	100	2.6															4	Slight	Slight	n.p.			Spielmann et al. (1996)
RK Blau		MD	100%, 10%, and ITC	-	n.p.	100	2.6															0	Nonirritant		n.p.			Spielmann et al. (1996)
Rubinrot Y		AP	100%, 10%, and ITC	-	n.p.	172																n.p.		Slight	5.3	Moderate	Moderate	Spielmann et al. (1996)
Rubinrot Y		HO	100%, 10%, and ITC	-	n.p.	172																4	Slight		n.p.			Spielmann et al. (1996)
Sacyclo		HO	100%, 10%, and ITC	-	n.p.	insoluble	n.s.															3.4	Slight	Slight	4.4	Slight	Slight	Spielmann et al. (1996)
Sacyclo		MD	100%, 10%, and ITC	-	n.p.	insoluble	n.s.															0	Nonirritant		3.3	Slight		Spielmann et al. (1996)
Sept		BD	100%, 10%, and ITC	-	n.p.	soluble	3															4	Severe	Severe	15.9	Severe	Severe	Spielmann et al. (1996)
Sept		HK	100%, 10%, and ITC	-	n.p.	soluble	3															10	Severe		19.8	Severe		Spielmann et al. (1996)
Trimethoxypropylsilane	1067-25-0	BD	100%, 10%, and ITC	-	n.p.	poorly soluble	n.s.															3.7	Slight	Slight	4.5	Slight	Severe	Spielmann et al. (1996)
Trimethoxypropylsilane	1067-25-0	AP	100%, 10%, and ITC	-	n.p.	poorly soluble	n.s.															3.9	Slight		13.7	Severe		Spielmann et al. (1996)
Trimethoxyoctylsilane	3069-40-7	HO	100%, 10%, and ITC	-	n.p.	insoluble	n.s.															7.9	Moderate	Moderate	8.4	Moderate	Severe	Spielmann et al. (1996)
Trimethoxyoctylsilane	3069-40-7	BG	100%, 10%, and ITC	-	n.p.	insoluble	n.s.															2.1	Slight		10	Severe		Spielmann et al. (1996)
Silan 165	29055-11-6	HO	100%, 10%, and ITC	-	n.p.	insoluble	n.s.															0.7	Nonirritant	Nonirritant	4.1	Slight	Moderate	Spielmann et al. (1996)
Silan 165	29055-11-6	WA	100%, 10%, and ITC	-	n.p.	insoluble	n.s.															0	Nonirritant		7.2	Moderate		Spielmann et al. (1996)
Silan 167	41453-78-5	WA	100%, 10%, and ITC	-	n.p.	soluble	n.s.															2.7	Slight	Slight	4.7	Slight	Slight	Spielmann et al. (1996)
Silan 167	41453-78-5	HO	100%, 10%, and ITC	-	n.p.	soluble	n.s.															0.1	Nonirritant		2.3	Slight		Spielmann et al. (1996)
Silan 253	18784-74-2	BD	100%, 10%, and ITC	-	n.p.	insoluble	<7															3	Severe	Severe	9.9	Severe	Severe	Spielmann et al. (1996)
Silan 253	18784-74-2	MD	100%, 10%, and ITC	-	n.p.	insoluble	<7															3	Severe		14.7	Severe		Spielmann et al. (1996)
Sodium bisulfite	7631-90-5	AP	100%, 10%, and ITC	-	n.p.	readily soluble	4.5															12.7	Severe	Severe	20	Severe	Severe	Spielmann et al. (1996)
Sodium bisulfite	7631-90-5	MD	100%, 10%, and ITC	-	n.p.	readily soluble	4.5															13.9	Severe		16.8	Severe		Spielmann et al. (1996)
Sodium sulfite	7757-83-7	AP	100%, 10%, and ITC	-	n.p.	250	10															13.2	Severe	Severe	16.1	Severe	Severe	Spielmann et al. (1996)
Sodium sulfite	7757-83-7	BG	100%, 10%, and ITC	-	n.p.	250	10															11.3	Severe		12.3	Severe		Spielmann et al. (1996)
Sodium cyanate	917-61-3	MD	100%, 10%, and ITC	-	n.p.	110	10.4															14.8	Severe	Severe	8.2	Moderate	Severe	Spielmann et al. (1996)
Sodium cyanate	917-61-3	WA	100%, 10%, and ITC	-	n.p.	110	10.4															10.5	Severe		10.7	Severe		Spielmann et al. (1996)
Sodium disilicate	13870-28-5	BG	100%, 10%, and ITC	-	n.p.	3.5	11.4															19.7	Severe	Severe	18.2	Severe	Severe	Spielmann et al. (1996)
Sodium disilicate	13870-28-5	HK	100%, 10%, and ITC	-	n.p.	3.5	11.4															20.7	Severe		16.6	Severe		Spielmann et al. (1996)

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Sodium hydrogen sulfate	7681-38-1	HK	100%, 10%, and ITC	-	n.p.	1080	1.1															18.8	Severe	Severe	19.2	Severe	Severe	Spielmann et al. (1996)
Sodium hydrogen sulfate	7681-38-1	WA	100%, 10%, and ITC	-	n.p.	1080	1.1															16.7	Severe		18.1	Severe		Spielmann et al. (1996)
Sodium lauryl ether sulfate	3088-31-1	BG	100%, 10%, and ITC	-	n.p.	soluble	8															10.5	Severe	Severe	17.9	Severe	Severe	Spielmann et al. (1996)
Sodium lauryl ether sulfate	3088-31-1	MD	100%, 10%, and ITC	-	n.p.	soluble	8															17.7	Severe		19	Severe		Spielmann et al. (1996)
Sodium monochloroacetate	3926-62-3	HO	100%, 10%, and ITC	-	n.p.	440	4.5															7.5	Moderate	Moderate	16.1	Severe	Severe	Spielmann et al. (1996)
Sodium monochloroacetate	3926-62-3	BD	100%, 10%, and ITC	-	n.p.	440	4.5															0	Nonirritant		10.8	Severe		Spielmann et al. (1996)
Sodiumpyrosulfite	7681-57-4	AP	100%, 10%, and ITC	-	n.p.	650	4.6															17.4	Severe	Severe	17.7	Severe	Severe	Spielmann et al. (1996)
Sodiumpyrosulfite	7681-57-4	BD	100%, 10%, and ITC	-	n.p.	650	4.6															12.6	Severe		11.6	Severe		Spielmann et al. (1996)
Sodiumpyrosulfite	7681-57-4	BG	100%, 10%, and ITC	-	n.p.	650	4.6															14.6	Severe		14.5	Severe		Spielmann et al. (1996)
4-((2-sulfatoethyl)sulfonyl)-aniline	2494-89-5	AP	100%, 10%, and ITC	-	n.p.	soluble	7															18	Severe	Severe	10.4	Severe	Severe	Spielmann et al. (1996)
4-((2-sulfatoethyl)sulfonyl)-aniline	2494-89-5	HK	100%, 10%, and ITC	-	n.p.	soluble	7															20.1	Severe		n.p.	Severe		Spielmann et al. (1996)
TA 01946 Alkylsilan		AP	100%, 10%, and ITC	-	n.p.	0.014	n.s.															7.6	Moderate	Severe	16.2	Severe	Severe	Spielmann et al. (1996)
TA 01946 Alkylsilan		HK	100%, 10%, and ITC	-	n.p.	0.014	n.s.															10	Severe		10	Severe		Spielmann et al. (1996)
Theophylline sodium acetate	8002-89-9	AP	100%, 10%, and ITC	-	n.p.	50	11															13.4	Severe	Severe	6.9	Moderate	Moderate	Spielmann et al. (1996)
Theophylline sodium acetate	8002-89-9	HO	100%, 10%, and ITC	-	n.p.	50	11															5.4	Moderate		n.p.	Severe		Spielmann et al. (1996)
Tocla		BD	100%, 10%, and ITC	-	n.p.	40	6															12.9	Severe	Severe	13.5	Severe	Severe	Spielmann et al. (1996)
Tocla		HK	100%, 10%, and ITC	-	n.p.	40	6															19.7	Severe		20.4	Severe		Spielmann et al. (1996)
Triisooctylamine	25549-16-0	BG	100%, 10%, and ITC	-	n.p.	0.5	7															0.8	Nonirritant	Nonirritant	14.1	Severe	Severe	Spielmann et al. (1996)
Triisooctylamine	25549-16-0	MD	100%, 10%, and ITC	-	n.p.	0.5	7															0	Nonirritant		4	Slight		Spielmann et al. (1996)
2,2,3-Trimethyl-3-Cyclo-pentene-1-acetaldehyde	4501-58-0	BG	100%, 10%, and ITC	-	n.p.	< 2.5	2.3															2.9	Slight	Slight	9.7	Severe	Severe	Spielmann et al. (1996)
2,2,3-Trimethyl-3-Cyclo-pentene-1-acetaldehyde	4501-58-0	AP	100%, 10%, and ITC	-	n.p.	< 2.5	2.3															2.3	Slight		14.7	Severe		Spielmann et al. (1996)
Trioxane	110-88-3	HK	100%, 10%, and ITC	-	n.p.	172	n.s.															9.25	Severe	Severe	18	Severe	Severe	Spielmann et al. (1996)
Trioxane	110-88-3	WA	100%, 10%, and ITC	-	n.p.	172	n.s.															13.4	Severe		17.8	Severe		Spielmann et al. (1996)
Wessalith Slurry		BG	100%, 10%, and ITC	-	n.p.	readily soluble	11															3.13	Slight	Severe	4.1	Slight	Severe	Spielmann et al. (1996)
Wessalith Slurry		WA	100%, 10%, and ITC	-	n.p.	readily soluble	11															10	Severe		15.7	Severe		Spielmann et al. (1996)
Xanthinol nicotinate	437-74-1	WA	100%, 10%, and ITC	-	n.p.	250	6															4	Slight	Severe	9	Severe	Severe	Spielmann et al. (1996)
Xanthinol nicotinate	437-74-1	HK	100%, 10%, and ITC	-	n.p.	250	6															11.3	Severe		17.4	Severe		Spielmann et al. (1996)

Substance Name	CASRN	Lab	*In Vitro* Conc. Tested	*In Vitro* Physical Form Tested	Purity (%)	Solubility*	pH	IS(A)[1]	IS(A) SD	IS(A) Classification	Overall IS(A) Classification	IS(B)[2]	IS(B) SD	IS(B) Classification	Overall IS(B) Classification	S-Score[3]	S-Score Classification	Overall S-Score Classification	Q-Score[4]	Q-Score Classification	Overall Q-Score Classification	IS(B)-10[5]	IS(B)-10 Class.	Overall IS(B)-10 Class.	IS(B)-100[5]	IS(B)-100 Class.	Overall IS(B)-100 Class.	Reference
Sodium lauryl sulfate	151-21-3		1%	Solution	n.p.		3.3					14.22		Severe														Vinardell and Macián (1994)
Tween 20	9005-64-5		100%	Liquid	n.p.		7.21					3.22		Slight														Vinardell and Macián (1994)

Abbreviations: CASRN = Chemical Abstract Service Registry Number, n.a. = not applicable, n.p. = not provided, Conc. = Concentration, IS = Irritation Score, ITC = Irritation Threshold Concentration, SD = standard deviation.

* Solubility = obtained from literature references; where available, expressed as g/mL

[1] IS(A) represents irritation scores that were calculated using the method described in Leupke (1985)

[2] IS(B) represents irritation scores that were calculated using a method similar to the one described in Kalweit et al. (1987, 1990)

[3] S-Score represents irritation scores that were calculated using the method described in Balls et al. (1995)

[4] Q-Score represents irritation scores that were calcualted using the method described in Balls et al. (1995)

[5] IS(B)-10 and IS(B)-100 represents irritation scores that were calculated using a method similar to the one described in Kalweit et al. (1987, 1990) where the *in vitro* score was obtained using a 10% or 100% concentration, respectively.

[6] The IS(B) analysis method does not yield an IS value greater than 21 and the calculated result of 23 for this substance is not possible. Based on results with the IS(A) analysis method (IS(A) = 17.8), the formulation would be classified as a severe irritant and was classified as such for the IS(B) analysis method.

[7] No information on the *in vitro* physical form of substances tested by Spielmann et al. (1996) were added since the tested form depended on the concentration being evaluated (10% or 100%). For information on the tested form *in vivo* see **Appendix D**.

Appendix C3

Data Sorted by Substance for IS(A) Analysis Method

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Substance Name	CASRN	Test Lab	*In Vitro* Concentration Tested	*In Vitro* Physical Form Tested	Purity (%)	Solubility	pH	IS(A)[1]	IS(A) SD	IS(A) Classification	Overall IS(A) Classification	Reference
Acetic acid	64-19-7	1	10%	Solution			2.4	16.5	2.89	Severe	Severe	Hagino et al. (1999)/Submitted Y. Ohno Data
Acetic acid	64-19-7	2	10%	Solution			2.4	16	3.92	Severe		Hagino et al. (1999)/Submitted Y. Ohno Data
Acetic acid	64-19-7	3	10%	Solution			2.4	17.25	6.24	Severe		Hagino et al. (1999)/Submitted Y. Ohno Data
Acetic acid	64-19-7	4	10%	Solution			2.4	19.5	1.91	Severe		Hagino et al. (1999)/Submitted Y. Ohno Data
Acetic acid	64-19-7	5	10%	Solution			2.4	17.5	4.04	Severe		Hagino et al. (1999)/Submitted Y. Ohno Data
Butanol	71-36-3	1	10%	Suspension			7.31	8.25	2.87	Moderate	Severe	Hagino et al. (1999)/Submitted Y. Ohno Data
Butanol	71-36-3	2	10%	Suspension			7.31	10.5	1.91	Severe		Hagino et al. (1999)/Submitted Y. Ohno Data
Butanol	71-36-3	3	10%	Suspension			7.31	12	0.00	Severe		Hagino et al. (1999)/Submitted Y. Ohno Data
Butanol	71-36-3	4	10%	Suspension			7.31	12	0.00	Severe		Hagino et al. (1999)/Submitted Y. Ohno Data
Butanol	71-36-3	5	10%	Suspension			7.31	5.75	1.50	Moderate		Hagino et al. (1999)/Submitted Y. Ohno Data
Cetyltrimethylammonium bromide	57-09-0	1	10%	Solution			5.89	19	1.63	Severe	Severe	Hagino et al. (1999)/Submitted Y. Ohno Data
Cetyltrimethylammonium bromide	57-09-0	2	10%	Solution			5.89	13.25	2.22	Severe		Hagino et al. (1999)/Submitted Y. Ohno Data
Cetyltrimethylammonium bromide	57-09-0	3	10%	Solution			5.89	18.5	1.91	Severe		Hagino et al. (1999)/Submitted Y. Ohno Data
Cetyltrimethylammonium bromide	57-09-0	4	10%	Solution			5.89	11	2.45	Severe		Hagino et al. (1999)/Submitted Y. Ohno Data
Cetyltrimethylammonium bromide	57-09-0	5	10%	Solution			5.89	9	0.00	Severe		Hagino et al. (1999)/Submitted Y. Ohno Data

Substance Name	CASRN	Test Lab	*In Vitro* Concentration Tested	*In Vitro* Physical Form Tested	Purity (%)	Solubility	pH	IS(A)[1]	IS(A) SD	IS(A) Classification	Overall IS(A) Classification	Reference
Chlorhexidine gluconate solution (20% solution)	18472-51-0	1	10%	Solution			6.56	19	1.63	Severe	Severe	Hagino et al. (1999)/Submitted Y. Ohno Data
Chlorhexidine gluconate solution (20% solution)	18472-51-0	2	10%	Solution			6.56	13.5	1.00	Severe		Hagino et al. (1999)/Submitted Y. Ohno Data
Chlorhexidine gluconate solution (20% solution)	18472-51-0	3	10%	Solution			6.56	16	2.45	Severe		Hagino et al. (1999)/Submitted Y. Ohno Data
Chlorhexidine gluconate solution (20% solution)	18472-51-0	4	10%	Solution			6.56	11.75	4.86	Severe		Hagino et al. (1999)/Submitted Y. Ohno Data
Chlorhexidine gluconate solution (20% solution)	18472-51-0	5	10%	Solution			6.56	9	0.00	Severe		Hagino et al. (1999)/Submitted Y. Ohno Data
Di(2-ethylhexyl) sodium sulfosuccinate	577-11-7	1	10%	Suspension			6.54	10	0.00	Severe	Severe	Hagino et al. (1999)/Submitted Y. Ohno Data
Di(2-ethylhexyl) sodium sulfosuccinate	577-11-7	2	10%	Suspension			6.54	10	1.63	Severe		Hagino et al. (1999)/Submitted Y. Ohno Data
Di(2-ethylhexyl) sodium sulfosuccinate	577-11-7	3	10%	Suspension			6.54	10.25	3.50	Severe		Hagino et al. (1999)/Submitted Y. Ohno Data
Di(2-ethylhexyl) sodium sulfosuccinate	577-11-7	4	10%	Suspension			6.54	12	0.00	Severe		Hagino et al. (1999)/Submitted Y. Ohno Data
Di(2-ethylhexyl) sodium sulfosuccinate	577-11-7	5	10%	Suspension			6.54	5	0.00	Moderate		Hagino et al. (1999)/Submitted Y. Ohno Data
Diisopropanolamine	110-97-4	1	10%	Solution			11.89	8.25	2.36	Moderate	Moderate	Hagino et al. (1999)/Submitted Y. Ohno Data
Diisopropanolamine	110-97-4	2	10%	Solution			11.89	8.5	4.04	Moderate		Hagino et al. (1999)/Submitted Y. Ohno Data
Diisopropanolamine	110-97-4	3	10%	Solution			11.89	9	1.15	Severe		Hagino et al. (1999)/Submitted Y. Ohno Data
Diisopropanolamine	110-97-4	4	10%	Solution			11.89	12	0.00	Severe		Hagino et al. (1999)/Submitted Y. Ohno Data
Diisopropanolamine	110-97-4	5	10%	Solution			11.89	5	0.00	Moderate		Hagino et al. (1999)/Submitted Y. Ohno Data

Substance Name	CASRN	Test Lab	*In Vitro* Concentration Tested	*In Vitro* Physical Form Tested	Purity (%)	Solubility	pH	IS(A)[1]	IS(A) SD	IS(A) Classification	Overall IS(A) Classification	Reference
Domiphen bromide	538-71-6	1	10%	Solution			6.22	19	0.00	Severe	Severe	Hagino et al. (1999)/Submitted Y. Ohno Data
Domiphen bromide	538-71-6	2	10%	Solution			6.22	15.25	2.36	Severe		Hagino et al. (1999)/Submitted Y. Ohno Data
Domiphen bromide	538-71-6	3	10%	Solution			6.22	14.75	1.50	Severe		Hagino et al. (1999)/Submitted Y. Ohno Data
Domiphen bromide	538-71-6	4	10%	Solution			6.22	12.25	2.36	Severe		Hagino et al. (1999)/Submitted Y. Ohno Data
Domiphen bromide	538-71-6	5	10%	Solution			6.22	9	1.22	Severe		Hagino et al. (1999)/Submitted Y. Ohno Data
Ethanol	64-17-5	1	10%	Solution			5.9	0	0.00	Nonirritant	Slight	Hagino et al. (1999)/Submitted Y. Ohno Data
Ethanol	64-17-5	2	10%	Solution			5.9	1.25	2.50	Slight		Hagino et al. (1999)/Submitted Y. Ohno Data
Ethanol	64-17-5	3	10%	Solution			5.9	10.5	1.91	Severe		Hagino et al. (1999)/Submitted Y. Ohno Data
Ethanol	64-17-5	4	10%	Solution			5.9	1.5	1.73	Slight		Hagino et al. (1999)/Submitted Y. Ohno Data
Ethanol	64-17-5	5	10%	Solution			5.9	1.25	2.50	Slight		Hagino et al. (1999)/Submitted Y. Ohno Data
Ethanol	64-17-5		10%	Solution			7.2	4		Slight		Kojima et al. (1995)
Ethanol	64-17-5	1	100%	Liquid				18.75	3.30	Severe	Severe	Hagino et al. (1999)/Submitted Y. Ohno Data
Ethanol	64-17-5	2	100%	Liquid				16	2.45	Severe		Hagino et al. (1999)/Submitted Y. Ohno Data
Ethanol	64-17-5	3	100%	Liquid				11.5	1.00	Severe		Hagino et al. (1999)/Submitted Y. Ohno Data
Ethanol	64-17-5	4	100%	Liquid				17	0.00	Severe		Hagino et al. (1999)/Submitted Y. Ohno Data
Ethanol	64-17-5	5	100%	Liquid				10.5	1.73	Severe		Hagino et al. (1999)/Submitted Y. Ohno Data

Substance Name	CASRN	Test Lab	*In Vitro* Concentration Tested	*In Vitro* Physical Form Tested	Purity (%)	Solubility	pH	IS(A)[1]	IS(A) SD	IS(A) Classification	Overall IS(A) Classification	Reference
Glycolic acid	79-14-1	1	10%	Solution			1.76	19.5	1.00	Severe	Severe	Hagino et al. (1999)/Submitted Y. Ohno Data
Glycolic acid	79-14-1	2	10%	Solution			1.76	20	1.15	Severe		Hagino et al. (1999)/Submitted Y. Ohno Data
Glycolic acid	79-14-1	3	10%	Solution			1.76	17.75	3.95	Severe		Hagino et al. (1999)/Submitted Y. Ohno Data
Glycolic acid	79-14-1	4	10%	Solution			1.76	12.25	2.36	Severe		Hagino et al. (1999)/Submitted Y. Ohno Data
Glycolic acid	79-14-1	5	10%	Solution			1.76	12.75	2.50	Severe		Hagino et al. (1999)/Submitted Y. Ohno Data
Lactic acid	50-21-5	1	10%	Solution			1.94	20.5	1.00	Severe	Severe	Hagino et al. (1999)/Submitted Y. Ohno Data
Lactic acid	50-21-5	2	10%	Solution			1.94	14.25	2.06	Severe		Hagino et al. (1999)/Submitted Y. Ohno Data
Lactic acid	50-21-5	3	10%	Solution			1.94	19.5	1.91	Severe		Hagino et al. (1999)/Submitted Y. Ohno Data
Lactic acid	50-21-5	4	10%	Solution			1.94	18.5	1.91	Severe		Hagino et al. (1999)/Submitted Y. Ohno Data
Lactic acid	50-21-5	5	10%	Solution			1.94	10.25	2.50	Severe		Hagino et al. (1999)/Submitted Y. Ohno Data
Lactic acid	50-21-5	1	100%	Liquid				21	0.00	Severe	Severe	Hagino et al. (1999)/Submitted Y. Ohno Data
Lactic acid	50-21-5	2	100%	Liquid				6.25	2.50	Moderate		Hagino et al. (1999)/Submitted Y. Ohno Data
Lactic acid	50-21-5	3	100%	Liquid				16	1.15	Severe		Hagino et al. (1999)/Submitted Y. Ohno Data
Lactic acid	50-21-5	4	100%	Liquid				15.25	2.50	Severe		Hagino et al. (1999)/Submitted Y. Ohno Data
Lactic acid	50-21-5	5	100%	Liquid				11.5	2.89	Severe		Hagino et al. (1999)/Submitted Y. Ohno Data

Substance Name	CASRN	Test Lab	*In Vitro* Concentration Tested	*In Vitro* Physical Form Tested	Purity (%)	Solubility	pH	IS(A)[1]	IS(A) SD	IS(A) Classification	Overall IS(A) Classification	Reference
Monoethanolamine	141-43-5	1	10%	Solution			12.58	12	0.00	Severe	Severe	Hagino et al. (1999)/Submitted Y. Ohno Data
Monoethanolamine	141-43-5	2	10%	Solution			12.58	12	0.00	Severe		Hagino et al. (1999)/Submitted Y. Ohno Data
Monoethanolamine	141-43-5	3	10%	Solution			12.58	12	0.00	Severe		Hagino et al. (1999)/Submitted Y. Ohno Data
Monoethanolamine	141-43-5	4	10%	Solution			12.58	12	0.00	Severe		Hagino et al. (1999)/Submitted Y. Ohno Data
Monoethanolamine	141-43-5	5	10%	Solution			12.58	12	0.00	Severe		Hagino et al. (1999)/Submitted Y. Ohno Data
Oil/Water Emulsion-HZA			100%	Solution				0		Nonirritant	Nonirritant	Gettings et al. (1994)
Oil/Water Emulsion-HZC			100%	Solution				0.283		Nonirritant	Nonirritant	Gettings et al. (1994)
Oil/Water Emulsion-HZE			100%	Solution				0.533		Nonirritant	Nonirritant	Gettings et al. (1994)
Oil/Water Emulsion-HZF			100%	Solution				7.33		Moderate	Moderate	Gettings et al. (1994)
Oil/Water Emulsion-HZH			100%	Solution				17.8		Severe	Severe	Gettings et al. (1994)
Oil/Water Emulsion-HZI			100%	Solution				1.97		Slight	Slight	Gettings et al. (1994)
Oil/Water Emulsion-HZJ			100%	Solution				0.917		Nonirritant	Nonirritant	Gettings et al. (1994)
Oil/Water Emulsion-HZL			100%	Solution				4.83		Slight	Slight	Gettings et al. (1994)
Oil/Water Emulsion-HZM			100%	Solution				8.33		Moderate	Moderate	Gettings et al. (1994)
Oil/Water Emulsion-HZN			100%	Solution				3.33		Slight	Slight	Gettings et al. (1994)
Oil/Water Emulsion-HZO			100%	Solution				0.5		Nonirritant	Nonirritant	Gettings et al. (1994)
Oil/Water Emulsion-HZR			100%	Solution				10.6		Severe	Severe	Gettings et al. (1994)
Oil/Water Emulsion-HZS			100%	Solution				11.6		Severe	Severe	Gettings et al. (1994)
Oil/Water Emulsion-HZT			100%	Solution				4.1		Slight	Slight	Gettings et al. (1994)
Oil/Water Emulsion-HZU			100%	Solution				0		Nonirritant	Nonirritant	Gettings et al. (1994)
Oil/Water Emulsion-HZV			100%	Solution				0.6		Nonirritant	Nonirritant	Gettings et al. (1994)
Oil/Water Emulsion-HZW			100%	Solution				0.167		Nonirritant	Nonirritant	Gettings et al. (1994)
Oil/Water Emulsion-HZY			100%	Solution				17		Severe	Severe	Gettings et al. (1994)

Substance Name	CASRN	Test Lab	*In Vitro* Concentration Tested	*In Vitro* Physical Form Tested	Purity (%)	Solubility	pH	IS(A)[1]	IS(A) SD	IS(A) Classification	Overall IS(A) Classification	Reference
Potassium laurate	10124-65-9	1	10%	Solution			10.49	20	1.15	Severe	Severe	Hagino et al. (1999)/Submitted Y. Ohno Data
Potassium laurate	10124-65-9	2	10%	Solution			10.49	13.25	2.50	Severe		Hagino et al. (1999)/Submitted Y. Ohno Data
Potassium laurate	10124-65-9	3	10%	Solution			10.49	12	0.00	Severe		Hagino et al. (1999)/Submitted Y. Ohno Data
Potassium laurate	10124-65-9	4	10%	Solution			10.49	12	0.00	Severe		Hagino et al. (1999)/Submitted Y. Ohno Data
Potassium laurate	10124-65-9	5	10%	Solution			10.49	19.33	0.82	Severe		Hagino et al. (1999)/Submitted Y. Ohno Data
Potassium laurate	10124-65-9		10%	Solution	98%		9.4	14.3		Severe		Kojima et al. (1995)
Sodium lauryl sulfate	151-21-3		10%	Solution	98%		5.4	7.5		Moderate	Severe	Kojima et al. (1995)
Stearyltrimethylammonium chloride	15461-40-2	1	10%	Solution			4.24	16.75	2.06	Severe	Severe	Hagino et al. (1999)/Submitted Y. Ohno Data
Stearyltrimethylammonium chloride	15461-40-2	2	10%	Solution			4.24	13	2.00	Severe		Hagino et al. (1999)/Submitted Y. Ohno Data
Stearyltrimethylammonium chloride	15461-40-2	3	10%	Solution			4.24	15.75	3.50	Severe		Hagino et al. (1999)/Submitted Y. Ohno Data
Stearyltrimethylammonium chloride	15461-40-2	4	10%	Solution			4.24	13.5	1.00	Severe		Hagino et al. (1999)/Submitted Y. Ohno Data
Stearyltrimethylammonium chloride	15461-40-2	5	10%	Solution			4.24	9	0.00	Severe		Hagino et al. (1999)/Submitted Y. Ohno Data
Stearyltrimethylammonium chloride	15461-40-2		10%	Solution			5.5	19.3		Severe		Kojima et al. (1995)
Surfactant Based Formulation 1-HZA			10%	Solution				7.8		Moderate	Moderate	Gettings et al. (1996)
Surfactant Based Formulation 2-HZB			10%	Solution				4.8		Slight	Slight	Gettings et al. (1996)
Surfactant Based Formulation 3-HZC			10%	Solution				9.5		Severe	Severe	Gettings et al. (1996)
Surfactant Based Formulation 4-HZD			10%	Solution				5.2		Moderate	Moderate	Gettings et al. (1996)
Surfactant Based Formulation 5-HZE			10%	Solution				3.8		Slight	Slight	Gettings et al. (1996)
Surfactant Based Formulation 6-HZF			10%	Solution				8.3		Moderate	Moderate	Gettings et al. (1996)
Surfactant Based Formulation 7-HZG			10%	Solution				6.3		Moderate	Moderate	Gettings et al. (1996)
Surfactant Based Formulation 8-HZH			10%	Solution				1.3		Slight	Slight	Gettings et al. (1996)
Surfactant Based Formulation 9-HZI			10%	Solution				9.3		Severe	Severe	Gettings et al. (1996)

Substance Name	CASRN	Test Lab	*In Vitro* Concentration Tested	*In Vitro* Physical Form Tested	Purity (%)	Solubility	pH	IS(A)[1]	IS(A) SD	IS(A) Classification	Overall IS(A) Classification	Reference
Surfactant Based Formulation 10-HZJ			10%	Solution				2.2		Slight	Slight	Gettings et al. (1996)
Surfactant Based Formulation 11-HZK			10%	Solution				8.8		Moderate	Moderate	Gettings et al. (1996)
Surfactant Based Formulation 12-HZL			10%	Solution				9.6		Severe	Severe	Gettings et al. (1996)
Surfactant Based Formulation 13-HZM			10%	Solution				4.1		Slight	Slight	Gettings et al. (1996)
Surfactant Based Formulation 14-HZN			10%	Solution				6.1		Moderate	Moderate	Gettings et al. (1996)
Surfactant Based Formulation 15-HZP			10%	Solution				4.7		Slight	Slight	Gettings et al. (1996)
Surfactant Based Formulation 16-HZQ			10%	Solution				4.9		Slight	Slight	Gettings et al. (1996)
Surfactant Based Formulation 17-HZR			10%	Solution				7.7		Moderate	Moderate	Gettings et al. (1996)
Surfactant Based Formulation 18-HZS			10%	Solution				8.8		Moderate	Moderate	Gettings et al. (1996)
Surfactant Based Formulation 19-HZT			10%	Solution				0.2		Nonirritant	Nonirritant	Gettings et al. (1996)
Surfactant Based Formulation 20-HZU			10%	Solution				3.7		Slight	Slight	Gettings et al. (1996)
Surfactant Based Formulation 21-HZV			10%	Solution				7.7		Moderate	Moderate	Gettings et al. (1996)
Surfactant Based Formulation 22-HZW			10%	Solution				7.8		Moderate	Moderate	Gettings et al. (1996)
Surfactant Based Formulation 23-HZX			10%	Solution				9		Severe	Severe	Gettings et al. (1996)
Surfactant Based Formulation 24-HZY			10%	Solution				8.7		Moderate	Moderate	Gettings et al. (1996)
Surfactant Based Formulation 25-HZZ			10%	Solution				0.7		Nonirritant	Nonirritant	Gettings et al. (1996)
Triethanolamine	102-71-6		10%	Solution				10.75		Severe	Slight	Bagley et al. (1992)
Triethanolamine	102-71-6	1	10%	Solution			11.26	1.5	2.38	Slight		Hagino et al. (1999)/Submitted Y. Ohno Data
Triethanolamine	102-71-6	2	10%	Solution			11.26	3.75	4.79	Slight		Hagino et al. (1999)/Submitted Y. Ohno Data
Triethanolamine	102-71-6	3	10%	Solution			11.26	11	1.15	Severe		Hagino et al. (1999)/Submitted Y. Ohno Data
Triethanolamine	102-71-6	4	10%	Solution			11.26	6	1.63	Moderate		Hagino et al. (1999)/Submitted Y. Ohno Data
Triethanolamine	102-71-6	5	10%	Solution			11.26	2.5	2.89	Slight		Hagino et al. (1999)/Submitted Y. Ohno Data

Substance Name	CASRN	Test Lab	*In Vitro* Concentration Tested	*In Vitro* Physical Form Tested	Purity (%)	Solubility	pH	IS(A)[1]	IS(A) SD	IS(A) Classification	Overall IS(A) Classification	Reference
Triethanolamine	102-71-6	1	100%	Liquid				5	0.00	Moderate	Moderate	Hagino et al. (1999)/Submitted Y. Ohno Data
Triethanolamine	102-71-6	2	100%	Liquid				6.75	3.50	Moderate		Hagino et al. (1999)/Submitted Y. Ohno Data
Triethanolamine	102-71-6	3	100%	Liquid				11.5	1.00	Severe		Hagino et al. (1999)/Submitted Y. Ohno Data
Triethanolamine	102-71-6	4	100%	Liquid				12	0.00	Severe		Hagino et al. (1999)/Submitted Y. Ohno Data
Triethanolamine	102-71-6	5	100%	Liquid				6.75	3.50	Moderate		Hagino et al. (1999)/Submitted Y. Ohno Data
Triton X-100	9002-93-1		1%	Solution				9		Severe	Severe	Bagley et al. (1992)
Triton X-100	9002-93-1		10%	Solution			5.75	5		Moderate	Moderate	Kojima et al. (1995)

Abbreviations: CASRN = Chemical Abstract Service Registry Number, SD = Standard Deviation.

[1] IS(A) represents irritation scores that were calculated using the method described in Leupke (1985).

Appendix C4

Data Sorted by Substance for IS(A)-10 Analysis Method

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Substance Name	CASRN	*In Vitro* Conc. Tested	*In Vitro* Physical Form Tested	Purity (%)	Solubility	pH	IS(A)-10[1]	IS(A)-10 Classification	Reference
Surfactant Based Formulation 1-HZA		10%	Solution				7.8	Moderate	Gettings et al. (1996)
Surfactant Based Formulation 2-HZB		10%	Solution				4.8	Slight	Gettings et al. (1996)
Surfactant Based Formulation 3-HZC		10%	Solution				9.5	Severe	Gettings et al. (1996)
Surfactant Based Formulation 4-HZD		10%	Solution				5.2	Moderate	Gettings et al. (1996)
Surfactant Based Formulation 5-HZE		10%	Solution				3.8	Slight	Gettings et al. (1996)
Surfactant Based Formulation 6-HZF		10%	Solution				8.3	Moderate	Gettings et al. (1996)
Surfactant Based Formulation 7-HZG		10%	Solution				6.3	Moderate	Gettings et al. (1996)

Substance Name	CASRN	*In Vitro* Conc. Tested	*In Vitro* Physical Form Tested	Purity (%)	Solubility	pH	IS(A)-10[1]	IS(A)-10 Classification	Reference
Surfactant Based Formulation 8-HZH		10%	Solution				1.3	Slight	Gettings et al. (1996)
Surfactant Based Formulation 9-HZI		10%	Solution				9.3	Severe	Gettings et al. (1996)
Surfactant Based Formulation 10-HZJ		10%	Solution				2.2	Slight	Gettings et al. (1996)
Surfactant Based Formulation 11-HZK		10%	Solution				8.8	Moderate	Gettings et al. (1996)
Surfactant Based Formulation 12-HZL		10%	Solution				9.6	Severe	Gettings et al. (1996)
Surfactant Based Formulation 13-HZM		10%	Solution				4.1	Slight	Gettings et al. (1996)
Surfactant Based Formulation 14-HZN		10%	Solution				6.1	Moderate	Gettings et al. (1996)

Substance Name	CASRN	*In Vitro* Conc. Tested	*In Vitro* Physical Form Tested	Purity (%)	Solubility	pH	IS(A)-10[1]	IS(A)-10 Classification	Reference
Surfactant Based Formulation 15-HZP		10%	Solution				4.7	Slight	Gettings et al. (1996)
Surfactant Based Formulation 16-HZQ		10%	Solution				4.9	Slight	Gettings et al. (1996)
Surfactant Based Formulation 17-HZR		10%	Solution				7.7	Moderate	Gettings et al. (1996)
Surfactant Based Formulation 18-HZS		10%	Solution				8.8	Moderate	Gettings et al. (1996)
Surfactant Based Formulation 19-HZT		10%	Solution				0.2	Nonirritant	Gettings et al. (1996)
Surfactant Based Formulation 20-HZU		10%	Solution				3.7	Slight	Gettings et al. (1996)
Surfactant Based Formulation 21-HZV		10%	Solution				7.7	Moderate	Gettings et al. (1996)

Substance Name	CASRN	*In Vitro* Conc. Tested	*In Vitro* Physical Form Tested	Purity (%)	Solubility	pH	IS(A)-10[1]	IS(A)-10 Classification	Reference
Surfactant Based Formulation 22-HZW		10%	Solution				7.8	Moderate	Gettings et al. (1996)
Surfactant Based Formulation 23-HZX		10%	Solution				9	Severe	Gettings et al. (1996)
Surfactant Based Formulation 24-HZY		10%	Solution				8.7	Moderate	Gettings et al. (1996)
Surfactant Based Formulation 25-HZZ		10%	Solution				0.7	Nonirritant	Gettings et al. (1996)

Abbreviation: CASRN: Chemical Abstracts Service Registy Number.

[1] IS(A)-10 represents irritation scores that were calculated using a method similar to the one described in Luepke (1985) where the *in vitro* score was obtained using a 10% concentration and where *in vivo* data were obtained at 100% concentration.

Appendix C5

Data Sorted by Substance for IS(A)-100 Analysis Method

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Substance Name	CASRN	Test Lab	*In Vitro* Conc. Tested	*In Vitro* Physical Form Tested	Purity (%)	Solubility	pH	IS(A)-100[1]	IS(A)-100 SD	IS(A)-100 Classification	Overall IS(A)-100 Classification	Reference
Ethanol	64-17-5	1	100%	Liquid				18.75	3.30	Nonirritant	Severe	Hagino et al. (1999)/Submitted Y. Ohno Data
Ethanol	64-17-5	2	100%	Liquid				16	2.45	Severe		Hagino et al. (1999)/Submitted Y. Ohno Data
Ethanol	64-17-5	3	100%	Liquid				11.5	1.00	Severe		Hagino et al. (1999)/Submitted Y. Ohno Data
Ethanol	64-17-5	4	100%	Liquid				17	0.00	Severe		Hagino et al. (1999)/Submitted Y. Ohno Data
Ethanol	64-17-5	5	100%	Liquid				10.5	1.73	Nonirritant		Hagino et al. (1999)/Submitted Y. Ohno Data
Lactic acid	50-21-5	1	100%	Liquid				21	0.00	Nonirritant	Severe	Hagino et al. (1999)/Submitted Y. Ohno Data
Lactic acid	50-21-5	2	100%	Liquid				6.25	2.50	Nonirritant		Hagino et al. (1999)/Submitted Y. Ohno Data
Lactic acid	50-21-5	3	100%	Liquid				16	1.15	Nonirritant		Hagino et al. (1999)/Submitted Y. Ohno Data
Lactic acid	50-21-5	4	100%	Liquid				15.25	2.50	Nonirritant		Hagino et al. (1999)/Submitted Y. Ohno Data
Lactic acid	50-21-5	5	100%	Liquid				11.5	2.89	Nonirritant		Hagino et al. (1999)/Submitted Y. Ohno Data
Oil/Water Emulsion-HZA			100%	Solution				0		Nonirritant	Nonirritant	Gettings et al. (1994)
Oil/Water Emulsion-HZC			100%	Solution				0.283		Nonirritant	Nonirritant	Gettings et al. (1994)
Oil/Water Emulsion-HZE			100%	Solution				0.533		Nonirritant	Nonirritant	Gettings et al. (1994)

Substance Name	CASRN	Test Lab	*In Vitro* Conc. Tested	*In Vitro* Physical Form Tested	Purity (%)	Solubility	pH	IS(A)-100[1]	IS(A)-100 SD	IS(A)-100 Classification	Overall IS(A)-100 Classification	Reference
Oil/Water Emulsion-HZF			100%	Solution				7.33		Moderate	Moderate	Gettings et al. (1994)
Oil/Water Emulsion-HZH			100%	Solution				17.8		Severe	Severe	Gettings et al. (1994)
Oil/Water Emulsion-HZI			100%	Solution				1.97		Slight	Slight	Gettings et al. (1994)
Oil/Water Emulsion-HZJ			100%	Solution				0.917		Nonirritant	Nonirritant	Gettings et al. (1994)
Oil/Water Emulsion-HZL			100%	Solution				4.83		Slight	Slight	Gettings et al. (1994)
Oil/Water Emulsion-HZM			100%	Solution				8.33		Moderate	Moderate	Gettings et al. (1994)
Oil/Water Emulsion-HZN			100%	Solution				3.33		Slight	Slight	Gettings et al. (1994)
Oil/Water Emulsion-HZO			100%	Solution				0.5		Nonirritant	Nonirritant	Gettings et al. (1994)
Oil/Water Emulsion-HZR			100%	Solution				10.6		Severe	Severe	Gettings et al. (1994)
Oil/Water Emulsion-HZS			100%	Solution				11.6		Severe	Severe	Gettings et al. (1994)
Oil/Water Emulsion-HZT			100%	Solution				4.1		Slight	Slight	Gettings et al. (1994)
Oil/Water Emulsion-HZU			100%	Solution				0		Nonirritant	Nonirritant	Gettings et al. (1994)

Substance Name	CASRN	Test Lab	*In Vitro* Conc. Tested	*In Vitro* Physical Form Tested	Purity (%)	Solubility	pH	IS(A)-100[1]	IS(A)-100 SD	IS(A)-100 Classification	Overall IS(A)-100 Classification	Reference
Oil/Water Emulsion-HZV			100%	Solution				0.6		Nonirritant	Nonirritant	Gettings et al. (1994)
Oil/Water Emulsion-HZW			100%	Solution				0.167		Nonirritant	Nonirritant	Gettings et al. (1994)
Oil/Water Emulsion-HZY			100%	Solution				17		Severe	Severe	Gettings et al. (1994)
Triethanolamine	102-71-6	1	100%	Liquid				5	0.00	Severe	Severe	Hagino et al. (1999)/Submitted Y. Ohno Data
Triethanolamine	102-71-6	2	100%	Liquid				6.75	3.50	Nonirritant		Hagino et al. (1999)/Submitted Y. Ohno Data
Triethanolamine	102-71-6	3	100%	Liquid				11.5	1.00	Nonirritant		Hagino et al. (1999)/Submitted Y. Ohno Data
Triethanolamine	102-71-6	4	100%	Liquid				12	0.00	Nonirritant		Hagino et al. (1999)/Submitted Y. Ohno Data
Triethanolamine	102-71-6	5	100%	Liquid				6.75	3.50	Nonirritant		Hagino et al. (1999)/Submitted Y. Ohno Data

Abbreviation: CASRN: Chemical Abstracts Service Registy Number, Conc.: concentration, SD: standard deviation.

[1] IS(A)-10 represents irritation scores that were calculated using a method similar to the one described in Luepke (1985) where the *in vitro* score was obtained using a 100% concentration and where *in vivo* results were obtained at 100% concentration.

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Appendix C6

Data Sorted by Substance for IS(B) Analysis Method

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Substance Name	CASRN	Test Lab	*In Vitro* Concentration Tested	*In Vitro* Physical Form Tested	Purity (%)	Solubility	pH	IS(B)[1]	IS(B) SD	IS(B) Classification	Overall IS(B) Classification	Reference
Acetic acid	64-19-7	2	100%	Liquid	>99			14.8		Severe	Severe	CEC (1991)
Acetic acid	64-19-7	3	100%	Liquid	>99			13.7		Severe		CEC (1991)
Acetic acid	64-19-7	4	100%	Liquid	>99			9.3		Severe		CEC (1991)
Acetic acid	64-19-7	2	10%	Solution	>99			20.2		Severe	Severe	CEC (1991)
Acetic acid	64-19-7	3	10%	Solution	>99			13.6		Severe		CEC (1991)
Acetic acid	64-19-7	4	10%	Solution	>99			10.2		Severe		CEC (1991)
Acetone	67-64-1		100%	Liquid	>99	water soluble		15.32	0.33	Severe	Severe	Gilleron et al. (1997)
Allyl alcohol	107-18-6		100%	Liquid				12.4	2.3	Severe	Severe	Gilleron et al. (1996)
2-Aminophemol	95-55-6		100%	Solid				0.8	0.7	Nonirritant	Nonirritant	Gilleron et al. (1996)
Ammonium nitrate	6484-52-2		100%	Solid	>99.9	water soluble		15.34	1.24	Severe	Severe	Gilleron et al. (1997)
Anthracene	120-12-7		100%	Solid				0	0	Nonirritant	Nonirritant	Gilleron et al. (1996)
L-Aspartic acid	70-47-3		100%	Solid	95	water soluble		1.06	1.2	Slight	Slight	Gilleron et al. (1997)
Benzalkonium chloride	8001-54-5		100%	Liquid	98	surfactant		14.8	0.53	Severe	Severe	Gilleron et al. (1997)
Benzalkonium chloride	8001-54-5		100%	Liquid	98	surfactant		15.05	0.27	Severe	Severe	Gilleron et al. (1997)
Benzalkonium chloride	8001-54-5		100%	Liquid	98	surfactant		15.14	0.25	Severe	Severe	Gilleron et al. (1997)
Benzalkonium chloride	8001-54-5	2	100%	Unknown	n.p.			14.5		Severe	Severe	CEC (1991)
Benzalkonium chloride	8001-54-5	3	100%	Unknown	n.p.			13.1		Severe		CEC (1991)
Benzalkonium chloride	8001-54-5	5	100%	Unknown	n.p.			5.8		Moderate		CEC (1991)
Benzalkonium chloride	8001-54-5	6	100%	Unknown	n.p.			6.9		Moderate		CEC (1991)
Benzalkonium chloride	8001-54-5	7	100%	Unknown	n.p.			13.3		Severe		CEC (1991)
Benzethonium chloride	121-54-0		100%	Solid	n.p.			15.4	3.1	Severe	Severe	Gilleron et al. (1996)

Substance Name	CASRN	Test Lab	*In Vitro* Concentration Tested	*In Vitro* Physical Form Tested	Purity (%)	Solubility	pH	IS(B)[1]	IS(B) SD	IS(B) Classification	Overall IS(B) Classification	Reference
Brij 35	9002-92-0	1	100%	Solid	>99			2.3		Slight	Slight	CEC (1991)
Brij 35	9002-92-0	2	100%	Solid	>99			4.3		Slight		CEC (1991)
Brij 35	9002-92-0	3	100%	Solid	>99			12.9		Severe		CEC (1991)
Brij 35	9002-92-0	4	100%	Solid	>99			4.4		Slight		CEC (1991)
Brij 35	9002-92-0	5	100%	Solid	>99			3.8		Slight		CEC (1991)
Brij 35	9002-92-0	6	100%	Solid	>99			2.6		Slight		CEC (1991)
Brij 35	9002-92-0	7	100%	Solid	>99			4		Slight		CEC (1991)
Butanol	71-36-3	1	100%	Liquid	99			11.7		Severe	Severe	CEC (1991)
Butanol	71-36-3	2	100%	Liquid	99			11.8		Severe		CEC (1991)
Butanol	71-36-3	3	100%	Liquid	99			12.6		Severe		CEC (1991)
Butanol	71-36-3	4	100%	Liquid	99			11.2		Severe		CEC (1991)
Butanol	71-36-3	5	100%	Liquid	99			3.9		Slight		CEC (1991)
Butanol	71-36-3	6	100%	Liquid	99			10.7		Severe		CEC (1991)
Butanol	71-36-3	7	100%	Liquid	99			9.9		Severe		CEC (1991)
Butanol	71-36-3	2	10%	Solution	99			14.2		Severe	Severe	CEC (1991)
Butanol	71-36-3	3	10%	Solution	99			4.8		Slight		CEC (1991)
Butanol	71-36-3	4	10%	Solution	99			12.5		Severe		CEC (1991)
2-Butoxyethyl acetate	112-07-2	1	100%	Liquid	99			4.6		Slight	Slight	CEC (1991)
2-Butoxyethyl acetate	112-07-2	2	100%	Liquid	99			5.3		Moderate		CEC (1991)
2-Butoxyethyl acetate	112-07-2	3	100%	Liquid	99			4.7		Slight		CEC (1991)
2-Butoxyethyl acetate	112-07-2	4	100%	Liquid	99			4.7		Slight		CEC (1991)
2-Butoxyethyl acetate	112-07-2	5	100%	Liquid	99			4		Slight		CEC (1991)
2-Butoxyethyl acetate	112-07-2	6	100%	Liquid	99			3.9		Slight		CEC (1991)
2-Butoxyethyl acetate	112-07-2	7	100%	Liquid	99			4.5		Slight		CEC (1991)

Substance Name	CASRN	Test Lab	*In Vitro* Concentration Tested	*In Vitro* Physical Form Tested	Purity (%)	Solubility	pH	IS(B)[1]	IS(B) SD	IS(B) Classification	Overall IS(B) Classification	Reference
2-Butoxyethyl acetate	112-07-2	2	10%	Solution	99			4.1		Slight	Slight	CEC (1991)
2-Butoxyethyl acetate	112-07-2	3	10%	Solution	99			0		Nonirritant		CEC (1991)
2-Butoxyethyl acetate	112-07-2	4	10%	Solution	99			3.2		Slight		CEC (1991)
Butyl acetate	123-86-4		100%	Liquid	99	water insoluble		17.21	1.84	Severe	Severe	Gilleron et al. (1997)
Gamma-butyrolactone	96-48-0		100%	Liquid				13.9	1.8	Severe	Severe	Gilleron et al. (1996)
Gamma-butyrolactone	96-48-0		100%	Liquid	>99	water soluble		19.39	0.83	Severe		Gilleron et al. (1997)
Captan 90 concentrate	133-06-2		100%	Solid	90	water soluble		15.07	0.27	Severe	Severe	Gilleron et al. (1997)
4-Carboxybenzaldehyde	619-66-9		100%	Solid	95	water insoluble		3.95	4.69	Slight	Slight	Gilleron et al. (1997)
Cetylpyridinium bromide	140-72-7		100%	Liquid	98	surfactant		12.68	1.52	Severe	Severe	Gilleron et al. (1997)
Cetylpyridinium bromide	140-72-7		100%	Liquid	98	surfactant		13.53	2.42	Severe	Severe	Gilleron et al. (1997)
Cetylpyridinium bromide	140-72-7		100%	Liquid	98	surfactant		14.6	0.43	Severe	Severe	Gilleron et al. (1997)
Chlorhexidine	55-56-1		100%	Solid	99.5	water insoluble		14.87	3.78	Severe	Severe	Gilleron et al. (1997)
Cyclohexanol	108-93-0		100%	Liquid	97	water soluble		18.96	0.1	Severe	Severe	Gilleron et al. (1997)
Cyclohexanone	108-94-1		100%	Liquid				14.5	3.8	Severe	Severe	Gilleron et al. (1996)
Deoxycholic acid, sodium salt	302-95-4		100%	Solid				9.7	5.8	Severe	Severe	Gilleron et al. (1996)
Diacetone alcohol	123-42-2		100%	Liquid				15.1	2.7	Severe	Severe	Gilleron et al. (1996)
Dibenzoyl-L-tartaric acid	2743-38-6		100%	Solid	np	water soluble		13.34	4.24	Severe	Severe	Gilleron et al. (1997)
Dibenzoyl-L-tartaric acid	2743-38-6		100%	Solid				4.2	2.5	Slight		Gilleron et al. (1996)
Dibenzyl phosphate	1623-08-1		100%	Solid	99.5	water insoluble		15.16	0.47	Severe	Severe	Gilleron et al. (1997)
Dibutyltin chloride	683-18-1	1	100%	Solid	97			11.6		Severe	Severe	CEC (1991)
Dibutyltin chloride	683-18-1	2	100%	Solid	97			10.8		Severe		CEC (1991)
Dibutyltin chloride	683-18-1	4	100%	Solid	97			12.6		Severe		CEC (1991)
Dibutyltin chloride	683-18-1	5	100%	Solid	97			5.1		Moderate		CEC (1991)
Dibutyltin chloride	683-18-1	6	100%	Solid	97			5		Moderate		CEC (1991)
Dibutyltin chloride	683-18-1	7	100%	Solid	97			13		Severe		CEC (1991)
2,6-Dichlorobenzoyl chloride	4659-45-4		100%	Liquid	99	water insoluble		10.74	1.74	Severe	Severe	Gilleron et al. (1997)
2,4-Dicholor-5-sulfamolyl-benzoic acid	2736-23-4		100%	Solid				3.8	2.2	Slight	Slight	Gilleron et al. (1996)
Dimethyl biguanidine	657-24-9		100%	Solid				8.4	2.2	Moderate	Moderate	Gilleron et al. (1996)

Substance Name	CASRN	Test Lab	*In Vitro* Concentration Tested	*In Vitro* Physical Form Tested	Purity (%)	Solubility	pH	IS(B)[1]	IS(B) SD	IS(B) Classification	Overall IS(B) Classification	Reference
2,2-Dimethylbutanoic acid	595-37-9		100%	Liquid	>99	water insoluble		15.31	0.24	Severe	Severe	Gilleron et al. (1997)
2,5-Dimethylhexanediol	110-03-2		100%	Solid	99.5	water insoluble		15.33	0.38	Severe	Severe	Gilleron et al. (1997)
Dimethyl sulfoxide	67-68-5		100%	Liquid				11.3	3.7	Severe	Severe	Gilleron et al. (1996)
Dimethyl sulfoxide	67-68-5	1	100%	Liquid	99.9			11.7		Severe	Severe	CEC (1991)
Dimethyl sulfoxide	67-68-5	2	100%	Liquid	99.9			10.9		Severe		CEC (1991)
Dimethyl sulfoxide	67-68-5	3	100%	Liquid	99.9			11.3		Severe		CEC (1991)
Dimethyl sulfoxide	67-68-5	4	100%	Liquid	99.9			4.1		Slight		CEC (1991)
Dimethyl sulfoxide	67-68-5	5	100%	Liquid	99.9			4.9		Slight		CEC (1991)
Dimethyl sulfoxide	67-68-5	6	100%	Liquid	99.9			7.3		Moderate		CEC (1991)
Dimethyl sulfoxide	67-68-5	7	100%	Liquid	99.9			11.4		Severe		CEC (1991)
Dimethyl sulfoxide	67-68-5	2	10%	Solution	99.9			4.4		Slight	Slight	CEC (1991)
Dimethyl sulfoxide	67-68-5	3	10%	Solution	99.9			4.1		Slight		CEC (1991)
Dimethyl sulfoxide	67-68-5	4	10%	Solution	99.9			4.1		Slight		CEC (1991)
EDTA dipotassium	25105-12-9		100%	Solid				0	0	Nonirritant	Nonirritant	Gilleron et al. (1996)
Ethanol	64-17-5		100%	Liquid				11.3	2.8	Severe	Severe	Gilleron et al. (1996)
Ethanol	64-17-5		100%	Liquid		water soluble		14.97	0.04	Severe		Gilleron et al. (1997)
2-Ethoxyethanol	110-80-5		100%	Liquid				10.5	2.7	Severe	Severe	Gilleron et al. (1996)
Ethyl acetate	141-78-6		100%	Liquid	99	water soluble		19.32	0.06	Severe	Severe	Gilleron et al. (1997)
2-Ethyl-1-hexanol	104-76-7		100%	Liquid	99	water soluble		12.71	2.96	Severe	Severe	Gilleron et al. (1997)
Ethyl-2-methylacetoacetate	609-14-3		100%	Liquid	ca. 97	water insoluble		12.94	2.94	Severe	Severe	Gilleron et al. (1997)
Ethyl trimethyl acetate	3938-95-2		100%	Liquid	99	water insoluble		13.82	2.73	Severe	Severe	Gilleron et al. (1997)
Ethylacetoacetate	141-97-9		100%	Liquid				10	3.2	Severe	Severe	Gilleron et al. (1996)
Fomesafen	72128-02-0		100%	Solid	97.5	water soluble		1.21	1.29	Slight	Slight	Gilleron et al. (1997)
Furan	110-00-9		100%	Liquid				5.5	1	Moderate	Moderate	Gilleron et al. (1996)
Gluconolactone	90-80-2		100%	Solid				4.6	3.2	Slight	Slight	Gilleron et al. (1996)
DL-Glutamic acid	19285-83-7		100%	Solid				0.7	1.2	Nonirritant	Nonirritant	Gilleron et al. (1996)
Glycerol	56-81-5		100%	Liquid	99.5	water soluble		14.78	0.75	Severe	Severe	Gilleron et al. (1997)

Substance Name	CASRN	Test Lab	*In Vitro* Concentration Tested	*In Vitro* Physical Form Tested	Purity (%)	Solubility	pH	IS(B)[1]	IS(B) SD	IS(B) Classification	Overall IS(B) Classification	Reference
Glycerol	56-81-5	1	100%	Liquid	>99			10.8		Severe	Severe	CEC (1991)
Glycerol	56-81-5	2	100%	Liquid	>99			11.3		Severe		CEC (1991)
Glycerol	56-81-5	3	100%	Liquid	>99			10.3		Severe		CEC (1991)
Glycerol	56-81-5	4	100%	Liquid	>99			4.8		Slight		CEC (1991)
Glycerol	56-81-5	5	100%	Liquid	>99			0		Nonirritant		CEC (1991)
Glycerol	56-81-5	6	100%	Liquid	>99			0		Nonirritant		CEC (1991)
Glycerol	56-81-5	7	100%	Liquid	>99			9.4		Severe		CEC (1991)
Glycerol	56-81-5	2	10%	Solution	>99			8.7		Moderate	Slight	CEC (1991)
Glycerol	56-81-5	3	10%	Solution	>99			4.4		Slight		CEC (1991)
Glycerol	56-81-5	4	10%	Solution	>99			3.6		Slight		CEC (1991)
3-Glycidopropyltrimethoxysilane	2530-83-8		100%	Liquid				4.3	1	Slight	Slight	Gilleron et al. (1996)
Hexadecyltrimethylammonium bromide	57-09-0		100%	Liquid				10.8	4.8	Severe	Severe	Gilleron et al. (1996)
Hexane	110-54-3		100%	Liquid				3.1	2.7	Slight	Slight	Gilleron et al. (1996)
n-Hexane	110-54-3	1	100%	Liquid	99			2.9		Slight	Slight	CEC (1991)
n-Hexane	110-54-3	2	100%	Liquid	99			5.4		Moderate		CEC (1991)
n-Hexane	110-54-3	3	100%	Liquid	99			4.2		Slight		CEC (1991)
n-Hexane	110-54-3	4	100%	Liquid	99			10.3		Severe		CEC (1991)
n-Hexane	110-54-3	5	100%	Liquid	99			2.3		Slight		CEC (1991)
n-Hexane	110-54-3	6	100%	Liquid	99			8.1		Moderate		CEC (1991)
n-Hexane	110-54-3	7	100%	Liquid	99			2.4		Slight		CEC (1991)
n-Hexane	110-54-3	2	10%	Solution	99			3.7		Slight	Severe	CEC (1991)
n-Hexane	110-54-3	3	10%	Solution	99			0		Nonirritant		CEC (1991)
n-Hexane	110-54-3	4	10%	Solution	99			10.1		Severe		CEC (1991)
Hexanol	111-27-3		100%	Liquid	98	water insoluble		17.56	0.4	Severe	Severe	Gilleron et al. (1997)

Substance Name	CASRN	Test Lab	*In Vitro* Concentration Tested	*In Vitro* Physical Form Tested	Purity (%)	Solubility	pH	IS(B)[1]	IS(B) SD	IS(B) Classification	Overall IS(B) Classification	Reference
Hydroalcoholic Formulation 1-5% Alcohol Containing			Undiluted	Solution				4.6		Slight	Slight	Gettings et al. (1991)
Hydroalcoholic Formulation 2-10% Alcohol Containing			Undiluted	Solution				5		Moderate	Moderate	Gettings et al. (1991)
Hydroalcoholic Formulation 3-15% Alcohol Containing			Undiluted	Solution				8.5		Moderate	Moderate	Gettings et al. (1991)
Hydroalcoholic Formulation 4-20% Alcohol Containing			Undiluted	Solution				5.3		Moderate	Moderate	Gettings et al. (1991)
Hydroalcoholic Formulation 6-40% Alcohol Containing			Undiluted	Solution				11.9		Severe	Severe	Gettings et al. (1991)
Hydroalcoholic Formulation 7-55% Alcohol Containing			Undiluted	Solution				12.8		Severe	Severe	Gettings et al. (1991)
Hydroalcoholic Formulation 8-65% Alcohol Containing			Undiluted	Solution				12.7		Severe	Severe	Gettings et al. (1991)
Hydroalcoholic Formulation 9-83% Alcohol Containing			Undiluted	Solution				13.8		Severe	Severe	Gettings et al. (1991)
Hydroalcoholic Formulation 10-90% Alcohol Containing			Undiluted	Solution				13.6		Severe	Severe	Gettings et al. (1991)
Imidazole	288-32-4		100%	Solid				18.7	0.9	Severe	Severe	Gilleron et al. (1996)
Imidazole	288-32-4		100%	Solid	99	water soluble		19.43	0.49	Severe		Gilleron et al. (1997)
Iminodibenzyl	94-19-9		100%	Solid				0	0	Nonirritant	Nonirritant	Gilleron et al. (1996)
Isobutanol	78-83-1		100%	Liquid	99.9	water insoluble		19.41	0.08	Severe	Severe	Gilleron et al. (1997)
Isopropanol	67-63-0		100%	Liquid	99.9	water soluble		14.8	0.21	Severe	Severe	Gilleron et al. (1997)
N-Lauroylsarcosine, sodium salt	7631-98-3		100%	Solid				12.7	4.3	Severe	Severe	Gilleron et al. (1996)
Laurylsulfobetaine	14933-08-5		100%	Uknown				8.3	1.2	Moderate	Moderate	Gilleron et al. (1996)
Magnesium carbonate	56378-72-4		100%	Solid				1.4	1.9	Slight	Slight	Gilleron et al. (1996)
Maneb	12427-38-2		100%	Solid	90	water soluble		0.16	0.24	Nonirritant	Nonirritant	Gilleron et al. (1997)
Methanol	67-56-1		100%	Liquid				12.2	3.3	Severe	Severe	Gilleron et al. (1996)
2-Methoxyethanol	109-86-4		100%	Liquid				14.5	0.7	Severe	Severe	Gilleron et al. (1996)
2-Methoxyethanol	109-86-4	1	100%	Liquid	99			9.7		Severe	Severe	CEC (1991)
2-Methoxyethanol	109-86-4	2	100%	Liquid	99			12.2		Severe		CEC (1991)
2-Methoxyethanol	109-86-4	3	100%	Liquid	99			12.1		Severe		CEC (1991)
2-Methoxyethanol	109-86-4	4	100%	Liquid	99			8.6		Moderate		CEC (1991)
2-Methoxyethanol	109-86-4	5	100%	Liquid	99			4.5		Slight		CEC (1991)
2-Methoxyethanol	109-86-4	6	100%	Liquid	99			0.8		Nonirritant		CEC (1991)
2-Methoxyethanol	109-86-4	7	100%	Liquid	99			3.1		Slight		CEC (1991)

Substance Name	CASRN	Test Lab	*In Vitro* Concentration Tested	*In Vitro* Physical Form Tested	Purity (%)	Solubility	pH	IS(B)[1]	IS(B) SD	IS(B) Classification	Overall IS(B) Classification	Reference
2-Methoxyethanol	109-86-4	2	10%	Solution	99			7		Moderate	Moderate	CEC (1991)
2-Methoxyethanol	109-86-4	3	10%	Solution	99			0		Nonirritant		CEC (1991)
2-Methoxyethanol	109-86-4	4	10%	Solution	99			3.1		Slight		CEC (1991)
Methyl acetate	79-20-9		100%	Liquid	98	water soluble		18.98	0.75	Severe	Severe	Gilleron et al. (1997)
Methyl cyanoacetate	105-34-0		100%	Liquid	99	water soluble		16.31	1.23	Severe	Severe	Gilleron et al. (1997)
Methyl cyclopentane	96-37-7		100%	Liquid	>99	water insoluble		17.14	1.63	Severe	Severe	Gilleron et al. (1997)
Methyl ethyl ketone	78-93-3		100%	Liquid	99	water soluble		18.35	2.52	Severe	Severe	Gilleron et al. (1997)
Methyl isobutyl ketone	108-10-1		100%	Liquid	98	water insoluble		17.75	2.2	Severe	Severe	Gilleron et al. (1997)
Methyl isobutyl ketone	108-10-1		100%	Liquid				10.5	1.5	Severe		Gilleron et al. (1996)
MYRJ 45			100%	Unknown				0.00	0.00	Nonirritant	Nonirritant	Gilleron et al. (1996)
1-Naphthalene acetic acid	86-87-3		100%	Solid	99	water soluble		7.46	2.37	Moderate	Moderate	Gilleron et al. (1997)
1-Naphthalene acetic acid, Na salt	61-31-4		100%	Solid	95	water soluble		15.16	0.49	Severe	Severe	Gilleron et al. (1997)
1-Nitropropane	108-03-2		100%	Liquid				2.8	2.7	Slight	Slight	Gilleron et al. (1996)
Octanol	111-87-5		100%	Liquid				9.8	1.7	Severe	Severe	Gilleron et al. (1996)
Octanol	111-87-5		100%	Liquid	>99	water insoluble		16.7	0.81	Severe		Gilleron et al. (1997)
Oil/Water Emulsion-HZA			Undiluted	Solution				1		Slight	Nonirritant	Gettings et al. (1994)
Oil/Water Emulsion-HZC			Undiluted	Solution				3		Slight	Nonirritant	Gettings et al. (1994)
Oil/Water Emulsion-HZE			Undiluted	Solution				3.67		Slight	Nonirritant	Gettings et al. (1994)
Oil/Water Emulsion-HZF			Undiluted	Solution				3.67		Slight	Nonirritant	Gettings et al. (1994)
Oil/Water Emulsion-HZH[2]			Undiluted	Solution				23		Severe	Nonirritant	Gettings et al. (1994)
Oil/Water Emulsion-HZI			Undiluted	Solution				0.333		Nonirritant	Nonirritant	Gettings et al. (1994)
Oil/Water Emulsion-HZJ			Undiluted	Solution				3		Slight	Nonirritant	Gettings et al. (1994)
Oil/Water Emulsion-HZL			Undiluted	Solution				10.3		Severe	Nonirritant	Gettings et al. (1994)
Oil/Water Emulsion-HZM			Undiluted	Solution				14.3		Severe	Nonirritant	Gettings et al. (1994)
Oil/Water Emulsion-HZN			Undiluted	Solution				3.67		Slight	Nonirritant	Gettings et al. (1994)
Oil/Water Emulsion-HZO			Undiluted	Solution				0		Nonirritant	Nonirritant	Gettings et al. (1994)
Oil/Water Emulsion-HZR			Undiluted	Solution				16.3		Severe	Nonirritant	Gettings et al. (1994)

Substance Name	CASRN	Test Lab	*In Vitro* Concentration Tested	*In Vitro* Physical Form Tested	Purity (%)	Solubility	pH	IS(B)[1]	IS(B) SD	IS(B) Classification	Overall IS(B) Classification	Reference
Oil/Water Emulsion-HZS			Undiluted	Solution				8.33		Moderate	Nonirritant	Gettings et al. (1994)
Oil/Water Emulsion-HZT			Undiluted	Solution				1		Slight	Nonirritant	Gettings et al. (1994)
Oil/Water Emulsion-HZU			Undiluted	Solution				1		Slight	Nonirritant	Gettings et al. (1994)
Oil/Water Emulsion-HZV			Undiluted	Solution				0		Nonirritant	Nonirritant	Gettings et al. (1994)
Oil/Water Emulsion-HZW			Undiluted	Solution				5		Moderate	Nonirritant	Gettings et al. (1994)
Oil/Water Emulsion-HZY			Undiluted	Solution				9.67		Severe	Nonirritant	Gettings et al. (1994)
Parafluoraniline	371-40-4		100%	Liquid	99	water insoluble		15.49	1.63	Severe	Severe	Gilleron et al. (1997)
2,4-Pentadione	123-54-6		100%	Liquid				8.8	3	Moderate	Moderate	Gilleron et al. (1996)
1-Phenyl-3-pyrazolidine	92-43-3		100%	Solid				0.5	0.4	Nonirritant	Nonirritant	Gilleron et al. (1996)
Polyethylene glycol 400	25322-68-3		100%	Liquid		surfactant		14.68	0.55	Severe	Severe	Gilleron et al. (1997)
Polyoxyethylene 23 lauryl ether			100%	Solid				1.5	2.6	Slight	Slight	Gilleron et al. (1996)
Potassium cyanate	590-28-3		100%	Solid	97	water soluble		14.27	1.15	Severe	Severe	Gilleron et al. (1997)
Promethazine HCl	58-33-3		100%	Solid	98	water soluble		6.27	1.41	Moderate	Severe	Gilleron et al. (1997)
Promethazine HCl	58-33-3		100%	Solid				13.9	2.1	Severe		Gilleron et al. (1996)
Propyl-4-hydroxybenzoate	94-13-3		100%	Solid				1.9	1	Slight	Slight	Gilleron et al. (1996)
Pyridine	110-86-1		100%	Liquid				15.8	3.6	Severe	Severe	Gilleron et al. (1996)
Pyridine	110-86-1		100%	Liquid	>99	water soluble		17.79	2.44	Severe		Gilleron et al. (1997)
Quinacrine	69-05-6		100%	Solid				6.5	2.2	Moderate	Moderate	Gilleron et al. (1996)
Quinacrine	69-05-6		100%	Solid		water soluble		7.29	0.6	Moderate		Gilleron et al. (1997)
Sodium lauryl sulfate	151-21-3	1	100%	Solid	98			11.4		Severe	Severe	CEC (1991)
Sodium lauryl sulfate	151-21-3	2	100%	Solid	98			10.3		Severe		CEC (1991)
Sodium lauryl sulfate	151-21-3	3	100%	Solid	98			13.9		Severe		CEC (1991)
Sodium lauryl sulfate	151-21-3	4	100%	Solid	98			4.8		Slight		CEC (1991)
Sodium lauryl sulfate	151-21-3	6	100%	Solid	98			11.1		Severe		CEC (1991)
Sodium lauryl sulfate	151-21-3	7	100%	Solid	98			9.7		Severe		CEC (1991)
Sodium lauryl sulfate	151-21-3	2	10%	Solution	98			18.4		Severe	Severe	CEC (1991)
Sodium lauryl sulfate	151-21-3	3	10%	Solution	98			14.1		Severe		CEC (1991)
Sodium lauryl sulfate	151-21-3	4	10%	Solution	98			5.1		Moderate		CEC (1991)

Substance Name	CASRN	Test Lab	*In Vitro* Concentration Tested	*In Vitro* Physical Form Tested	Purity (%)	Solubility	pH	IS(B)[1]	IS(B) SD	IS(B) Classification	Overall IS(B) Classification	Reference
Sodium lauryl sulfate	151-21-3		1%	Solution			3.3	14.22		Severe	Nonirritant	Vinardell and Macián (1994)
Sodium lauryl sulfate	151-21-3		100%	Liquid	98	surfactant		12.38	1.82	Severe	Severe	Gilleron et al. (1997)
Sodium lauryl sulfate	151-21-3		100%	Liquid	98	surfactant		15.05	0.29	Severe	Severe	Gilleron et al. (1997)
Sodium hydroxide	1310-73-2		100%	Liquid		water soluble		19.01	0.13	Severe	Severe	Gilleron et al. (1997)
Sodium hydroxide	1310-73-2		100%	Liquid		water soluble		20.56	0.08	Severe	Severe	Gilleron et al. (1997)
Sodium oxalate	62-76-0		100%	Solid	>99	water soluble		14.2	0.71	Severe	Severe	Gilleron et al. (1997)
Sodium perborate	10486-00-7		100%	Solid	98.6	water soluble		13.19	1.78	Severe	Severe	Gilleron et al. (1997)
Surfactant Based Formulation 1-HZA			10%	Solution				9.6		Severe	Nonirritant	Gettings et al. (1996)
Surfactant Based Formulation 2-HZB			10%	Solution				7.3		Moderate	Nonirritant	Gettings et al. (1996)
Surfactant Based Formulation 3-HZC			10%	Solution				15.3		Severe	Nonirritant	Gettings et al. (1996)
Surfactant Based Formulation 4-HZD			10%	Solution				8.7		Moderate	Nonirritant	Gettings et al. (1996)
Surfactant Based Formulation 5-HZE			10%	Solution				11.4		Severe	Nonirritant	Gettings et al. (1996)
Surfactant Based Formulation 6-HZF			10%	Solution				10.9		Severe	Nonirritant	Gettings et al. (1996)
Surfactant Based Formulation 7-HZG			10%	Solution				7.1		Moderate	Nonirritant	Gettings et al. (1996)
Surfactant Based Formulation 8-HZH			10%	Solution				3.5		Slight	Nonirritant	Gettings et al. (1996)
Surfactant Based Formulation 9-HZI			10%	Solution				15.2		Severe	Nonirritant	Gettings et al. (1996)
Surfactant Based Formulation 10-HZJ			10%	Solution				6.2		Moderate	Nonirritant	Gettings et al. (1996)
Surfactant Based Formulation 11-HZK			10%	Solution				9.4		Severe	Nonirritant	Gettings et al. (1996)
Surfactant Based Formulation 12-HZL			10%	Solution				12.4		Severe	Nonirritant	Gettings et al. (1996)
Surfactant Based Formulation 13-HZM			10%	Solution				2.7		Slight	Nonirritant	Gettings et al. (1996)
Surfactant Based Formulation 14-HZN			10%	Solution				8		Moderate	Nonirritant	Gettings et al. (1996)
Surfactant Based Formulation 15-HZP			10%	Solution				4.4		Slight	Nonirritant	Gettings et al. (1996)
Surfactant Based Formulation 16-HZQ			10%	Solution				4.2		Slight	Nonirritant	Gettings et al. (1996)
Surfactant Based Formulation 17-HZR			10%	Solution				5.3		Moderate	Nonirritant	Gettings et al. (1996)
Surfactant Based Formulation 18-HZS			10%	Solution				12.2		Severe	Nonirritant	Gettings et al. (1996)
Surfactant Based Formulation 19-HZT			10%	Solution				3.5		Slight	Nonirritant	Gettings et al. (1996)
Surfactant Based Formulation 20-HZU			10%	Solution				6.2		Moderate	Nonirritant	Gettings et al. (1996)

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Surfactant Based Formulation 21-HZV			10%	Solution				8.7		Moderate	Nonirritant	Gettings et al. (1996)
Surfactant Based Formulation 22-HZW			10%	Solution				5.1		Moderate	Nonirritant	Gettings et al. (1996)
Surfactant Based Formulation 23-HZX			10%	Solution				11.3		Severe	Nonirritant	Gettings et al. (1996)
Surfactant Based Formulation 24-HZY			10%	Solution				11.7		Severe	Nonirritant	Gettings et al. (1996)
Surfactant Based Formulation 25-HZZ			10%	Solution				1.1		Slight	Nonirritant	Gettings et al. (1996)
Tetraaminopyrimidine sulfate	5392-28-9		100%	Solid				0.5	0.9	Nonirritant	Slight	Gilleron et al. (1996)
Tetraaminopyrimidine sulfate	5392-28-9		100%	Solid	97	water insoluble		4.33	0.23	Slight		Gilleron et al. (1997)
Thiourea	62-56-6		100%	Solid				13.7	4.4	Severe	Severe	Gilleron et al. (1996)
Thiourea	62-56-6		100%	Solid	>99	water soluble		17.89	1.53	Severe		Gilleron et al. (1997)
Toluene	108-88-3		100%	Liquid	99	water soluble		16.09	1.62	Severe	Severe	Gilleron et al. (1997)
Toluene	108-88-3	1	100%	Liquid	99.9			8.8		Moderate	Severe	CEC (1991)
Toluene	108-88-3	2	100%	Liquid	99.9			14.8		Severe		CEC (1991)
Toluene	108-88-3	3	100%	Liquid	99.9			15.2		Severe		CEC (1991)
Toluene	108-88-3	4	100%	Liquid	99.9			11.5		Severe		CEC (1991)
Toluene	108-88-3	5	100%	Liquid	99.9			4.6		Slight		CEC (1991)
Toluene	108-88-3	6	100%	Liquid	99.9			3.1		Slight		CEC (1991)
Toluene	108-88-3	7	100%	Liquid	99.9			4.9		Slight		CEC (1991)
Triacetin	102-76-1	1	100%	Liquid	99			3.6		Slight	Slight	CEC (1991)
Triacetin	102-76-1	2	100%	Liquid	99			4.3		Slight		CEC (1991)
Triacetin	102-76-1	3	100%	Liquid	99			5.5		Moderate		CEC (1991)
Triacetin	102-76-1	4	100%	Liquid	99			4.4		Slight		CEC (1991)
Triacetin	102-76-1	5	100%	Liquid	99			3.3		Slight		CEC (1991)
Triacetin	102-76-1	6	100%	Liquid	99			4.3		Slight		CEC (1991)
Triacetin	102-76-1	7	100%	Liquid	99			3.1		Slight		CEC (1991)

Substance Name	CASRN	Test Lab	*In Vitro* Concentration Tested	*In Vitro* Physical Form Tested	Purity (%)	Solubility	pH	IS(B)[1]	IS(B) SD	IS(B) Classification	Overall IS(B) Classification	Reference
Triacetin	102-76-1	2	10%	Solution	99			13.6		Severe	Slight	CEC (1991)
Triacetin	102-76-1	3	10%	Solution	99			2		Slight		CEC (1991)
Triacetin	102-76-1	4	10%	Solution	99			3.3		Slight		CEC (1991)
Tributyltin chloride	1461-22-9	1	100%	Solid	96			6.7		Moderate	Moderate	CEC (1991)
Tributyltin chloride	1461-22-9	2	100%	Solid	96			8.9		Moderate		CEC (1991)
Tributyltin chloride	1461-22-9	3	100%	Solid	96			13.7		Severe		CEC (1991)
Tributyltin chloride	1461-22-9	4	100%	Solid	96			8.8		Moderate		CEC (1991)
Tributyltin chloride	1461-22-9	5	100%	Solid	96			7.4		Moderate		CEC (1991)
Tributyltin chloride	1461-22-9	6	100%	Solid	96			7.9		Moderate		CEC (1991)
Tributyltin chloride	1461-22-9	7	100%	Solid	96			6.6		Moderate		CEC (1991)
Tributyltin chloride	1461-22-9	2	10%	Solution	96			15.6		Severe	Severe	CEC (1991)
Tributyltin chloride	1461-22-9	3	10%	Solution	96			9.6		Severe		CEC (1991)
Tributyltin chloride	1461-22-9	4	10%	Solution	96			11.2		Severe		CEC (1991)
Trichloroacetic acid	76-03-9		100%	Liquid		water soluble		15.7	0.11	Severe	Severe	Gilleron et al. (1997)
Trichloroacetic acid	76-03-9		100%	Liquid		water soluble		15.72	0.15	Severe	Severe	Gilleron et al. (1997)
1,2,3-Trichloropropane	96-18-4		100%	Liquid				7.9	1.7	Moderate	Moderate	Gilleron et al. (1996)
1,2,4-Trichloropropane	95-63-6		100%	Liquid				4.5	2.9	Slight	Slight	Gilleron et al. (1996)
Triethanolamine	102-71-6		100%	Liquid				9.6	3.5	Severe	Severe	Gilleron et al. (1996)
Triethanolamine	102-71-6	1	100%	Liquid	97			8.6		Moderate	Severe	CEC (1991)
Triethanolamine	102-71-6	2	100%	Liquid	97			10.4		Severe		CEC (1991)
Triethanolamine	102-71-6	3	100%	Liquid	97			11.9		Severe		CEC (1991)
Triethanolamine	102-71-6	4	100%	Liquid	97			4.2		Slight		CEC (1991)
Triethanolamine	102-71-6	5	100%	Liquid	97			0		Nonirritant		CEC (1991)
Triethanolamine	102-71-6	6	100%	Liquid	97			3.7		Slight		CEC (1991)
Triethanolamine	102-71-6	7	100%	Liquid	97			7.5		Moderate		CEC (1991)

Substance Name	CASRN	Test Lab	*In Vitro* Concentration Tested	*In Vitro* Physical Form Tested	Purity (%)	Solubility	pH	IS(B)[1]	IS(B) SD	IS(B) Classification	Overall IS(B) Classification	Reference
Triethanolamine	102-71-6	2	10%	Solution	97			11.3		Severe	Slight	CEC (1991)
Triethanolamine	102-71-6	3	10%	Solution	97			2.8		Slight		CEC (1991)
Triethanolamine	102-71-6	4	10%	Solution	97			1.1		Slight		CEC (1991)
Triton X-100	9002-93-1		100%	Liquid	98	surfactant		10.94	0.8	Severe	Severe	Gilleron et al. (1997)
Triton X-100	9002-93-1		100%	Liquid	98	surfactant		13.73	0.48	Severe	Severe	Gilleron et al. (1997)
Triton X-155	9010-44-0		100%	Surfactant				3.9	2.3	Slight	Slight	Gilleron et al. (1996)
Tween 20	9005-64-5		100%	Liquid	98	surfactant		14.47	0.36	Severe	Severe	Gilleron et al. (1997)
Tween 20	9005-64-5		100%	Liquid			7.21	3.22		Slight		Vinardell and Macián (1994)

Abbreviation: CASRN = Chemical Abstract Service Registry Number, SD = standard deviation.

[1] IS(B) represents irritation scores that were calculated using a method similar to the one described in Kalweit et al. (1987, 1990).

[2] The IS(B) analysis method does not yield an IS value greater than 21 and the calculated result of 23 for this substance is not possible. Based on results with the IS(A) analysis method (IS(A) = 17.8) in the same report, the formulation would be classified as a severe irritant and was classified as such for the IS(B) analysis method.

Appendix C7

Data Sorted by Substance for IS(B)-10 Analysis Method

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Substance Name	CASRN	Test Lab	*In Vitro* Concentration Tested	*In Vitro* Physical Form Tested	Purity (%)	Solubility[1]	pH	IS(B)-10[2]	IS(B)-10 Classification	Overall IS(B)-10 Classification	Reference
7-Acetoxyheptanal		MD	10%	Unknown		insoluble	n.s.	3.1	Slight	Slight	Spielmann et al. (1996)
7-Acetoxyheptanal		WA	10%	Unknown		insoluble	n.s.	0	Nonirritant		Spielmann et al. (1996)
n-Acetyl-Methionine	1115-47-5	MD	10%	Solid		83	2.2	13.6	Severe	Severe	Spielmann et al. (1996)
n-Acetyl-Methionine	1115-47-5	WA	10%	Solid		83	2.2	6.1	Moderate		Spielmann et al. (1996)
Ambuphylline	5634-34-4	BG	10%	Solid		600	9	10.7	Severe	Severe	Spielmann et al. (1996)
Ambuphylline	5634-34-4	MD	10%	Solid		600	9	15.8	Severe		Spielmann et al. (1996)
4-Amino-5-methoxy-2-methylbenzenesulfonic acid	6471-78-9	AP	10%	Unknown		3	1.5	14.8	Severe	Moderate	Spielmann et al. (1996)
4-Amino-5-methoxy-2-methylbenzenesulfonic acid	6471-78-9	WA	10%	Unknown		3	1.5	7	Moderate		Spielmann et al. (1996)
4-Amino-5-methoxy-2-methylbenzenesulfonic acid	6471-78-9	BG	10%	Unknown		3	1.5	7.6	Moderate		Spielmann et al. (1996)
Ammonium persulfate	7727-54-0	HO	10%	Solid		560	1.5	4.4	Slight	Slight	Spielmann et al. (1996)
Ammonium persulfate	7727-54-0	WA	10%	Solid		560	1.5	n.p.			Spielmann et al. (1996)

Substance Name	CASRN	Test Lab	*In Vitro* Concentration Tested	*In Vitro* Physical Form Tested	Purity (%)	Solubility[1]	pH	IS(B)-10[2]	IS(B)-10 Classification	Overall IS(B)-10 Classification	Reference
Anisole	100-66-3	AP	10%	Liquid		insoluble	n.s.	7.3	Moderate	Moderate	Spielmann et al. (1996)
Anisole	100-66-3	HK	10%	Liquid		insoluble	n.s.	0	Nonirritant		Spielmann et al. (1996)
B 25		BG	10%	Unknown		insoluble	n.s.	0	Nonirritant	Nonirritant	Spielmann et al. (1996)
B 25		WA	10%	Unknown		insoluble	n.s.	0	Nonirritant		Spielmann et al. (1996)
n-Butanal	123-72-8	HK	10%	Liquid		71	<7	1.2	Slight	Moderate	Spielmann et al. (1996)
n-Butanal	123-72-8	HO	10%	Liquid		71	<7	6.7	Moderate		Spielmann et al. (1996)
n-Butanol	71-36-3	BD	10%	Liquid		79	7	9.6	Severe	Severe	Spielmann et al. (1996)
n-Butanol	71-36-3	HK	10%	Liquid		79	7	18.3	Severe		Spielmann et al. (1996)
Butyl carbamate	592-35-8	BD	10%	Solid		1	n.s.	0	Nonirritant	Severe	Spielmann et al. (1996)
Butyl carbamate	592-35-8	MD	10%	Solid		1	n.s.	10.9	Severe		Spielmann et al. (1996)
Butyl carbamate	592-35-8	BG	10%	Solid		1	n.s.	9.5	Severe		Spielmann et al. (1996)

Substance Name	CASRN	Test Lab	*In Vitro* Concentration Tested	*In Vitro* Physical Form Tested	Purity (%)	Solubility[1]	pH	IS(B)-10[2]	IS(B)-10 Classification	Overall IS(B)-10 Classification	Reference
Caffeine sodium benzoate	8000-95-1	BD	10%	Solid		500	7	4.6	Slight	Moderate	Spielmann et al. (1996)
Caffeine sodium benzoate	8000-95-1	WA	10%	Solid		500	7	7.9	Moderate		Spielmann et al. (1996)
Caffeine sodium benzoate	8000-95-1	BG	10%	Solid		500	7	6.6	Moderate		Spielmann et al. (1996)
Caffeine sodium salicylate	8002-85-5	BG	10%	Solid		400	7	7.4	Moderate	Severe	Spielmann et al. (1996)
Caffeine sodium salicylate	8002-85-5	WA	10%	Solid		400	7	9.8	Severe		Spielmann et al. (1996)
Camphen	79-92-5	BG	10%	Solid		insoluble	7	2	Severe	Severe	Spielmann et al. (1996)
Camphen	79-92-5	HK	10%	Solid		insoluble	7	10	Severe		Spielmann et al. (1996)
Cerium-2-ethylhexanoate	24593-34-8	BG	10%	Unknown		n.s.	3	6.9	Moderate	Moderate	Spielmann et al. (1996)
Cerium-2-ethylhexanoate	24593-34-8	WA	10%	Unknown		n.s.	3	7.9	Moderate		Spielmann et al. (1996)
1-Chloroctane-8-ol		AP	10%	Unknown		insoluble	n.s.	6.8	Moderate	Moderate	Spielmann et al. (1996)
1-Chloroctane-8-ol		MD	10%	Unknown		insoluble	n.s.	4.3	Slight		Spielmann et al. (1996)

Substance Name	CASRN	Test Lab	*In Vitro* Concentration Tested	*In Vitro* Physical Form Tested	Purity (%)	Solubility[1]	pH	IS(B)-10[2]	IS(B)-10 Classification	Overall IS(B)-10 Classification	Reference
3-Cyclohexene-1-methanol	1679-51-2	BG	10%	Unknown		insoluble	n.s.	10.1	Severe	Severe	Spielmann et al. (1996)
3-Cyclohexene-1-methanol	1679-51-2	HO	10%	Unknown		insoluble	n.s.	11.8	Severe		Spielmann et al. (1996)
DC 8		BG	10%	Unknown		insoluble	n.s.	0	Nonirritant	Nonirritant	Spielmann et al. (1996)
DC 8		WA	10%	Unknown		insoluble	n.s.	0	Nonirritant		Spielmann et al. (1996)
1,4-Dibutoxy-benzene	104-36-9	HO	10%	Unknown		0.2	7	4.2	Slight	Slight	Spielmann et al. (1996)
1,4-Dibutoxy-benzene	104-36-9	WA	10%	Unknown		0.2	7	0	Nonirritant		Spielmann et al. (1996)
Diepoxid 126	2386-87-0	AP	10%	Liquid		insoluble	n.s.	6	Moderate	Moderate	Spielmann et al. (1996)
Diepoxid 126	2386-87-0	MD	10%	Liquid		insoluble	n.s.	8.6	Moderate		Spielmann et al. (1996)
Diepoxid 126	2386-87-0	BG	10%	Liquid		insoluble	n.s.	1.9	Slight		Spielmann et al. (1996)
2,5-Dimethylhexanediol	110-03-2	HK	10%	Solid		n.s.	n.s.	9.2	Severe	Severe	Spielmann et al. (1996)
2,5-Dimethylhexanediol	110-03-2	HO	10%	Solid		n.s.	n.s.	4.1	Slight		Spielmann et al. (1996)
2,5-Dimethylhexanediol	110-03-2	BG	10%	Solid		n.s.	n.s.				Spielmann et al. (1996)

Substance Name	CASRN	Test Lab	*In Vitro* Concentration Tested	*In Vitro* Physical Form Tested	Purity (%)	Solubility[1]	pH	IS(B)-10[2]	IS(B)-10 Classification	Overall IS(B)-10 Classification	Reference
3,6-Dimethyloctanol		BG	10%	Unknown		poorly soluble	7	0.3	Nonirritant	Nonirritant	Spielmann et al. (1996)
3,6-Dimethyloctanol		BD	10%	Unknown		poorly soluble	7	0	Nonirritant		Spielmann et al. (1996)
4,4-Dimethyl-3-oxo-pentanenitrile	59997-51-2	AP	10%	Solid		0.6	n.s.	4.3	Slight	Moderate	Spielmann et al. (1996)
4,4-Dimethyl-3-oxo-pentanenitrile	59997-51-2	WA	10%	Solid		0.6	n.s.	5.6	Moderate		Spielmann et al. (1996)
1-(2,6-dimethylphenoxy)-2-propanone	53012-41-2	HK	10%	Liquid		insoluble	5	18.9	Severe	Severe	Spielmann et al. (1996)
1-(2,6-dimethylphenoxy)-2-propanone	53012-41-2	WA	10%	Liquid		insoluble	5	2.6	Slight		Spielmann et al. (1996)
1-(2,6-dimethylphenoxy)-2-propanone	53012-41-2	BG	10%	Liquid		insoluble	5	0.75	Nonirritant		Spielmann et al. (1996)
Diphocars		HK	10%	Unknown		soluble	n.s.	18.3	Severe	Severe	Spielmann et al. (1996)
Diphocars		HO	10%	Unknown		soluble	n.s.	11.1	Severe		Spielmann et al. (1996)
1,2-Dodecanediol	1119-87-5	AP	10%	Solid		insoluble	n.s.	12.1	Severe	Slight	Spielmann et al. (1996)
1,2-Dodecanediol	1119-87-5	BG	10%	Solid		insoluble	n.s.	1.8	Slight		Spielmann et al. (1996)
1,2-Dodecanediol	1119-87-5	BG	10%	Solid		insoluble	n.s.	2.54	Slight		Spielmann et al. (1996)

Substance Name	CASRN	Test Lab	*In Vitro* Concentration Tested	*In Vitro* Physical Form Tested	Purity (%)	Solubility[1]	pH	IS(B)-10[2]	IS(B)-10 Classification	Overall IS(B)-10 Classification	Reference
DTPA Pentasodium salt	140-01-2	BG	10%	Unknown		readily soluble	11.5	15.66	Severe	Severe	Spielmann et al. (1996)
DTPA Pentasodium salt	140-01-2	WA	10%	Unknown		readily soluble	11.5	15.5	Severe		Spielmann et al. (1996)
Ede 140		WA	10%	Unknown		insoluble	n.s.	0	Nonirritant	Slight	Spielmann et al. (1996)
Ede 140		BD	10%	Unknown		insoluble	n.s.	3.4	Slight		Spielmann et al. (1996)
1,2-Epoxycyclooctane	286-62-4	MD	10%	Solid		<2.5	4.5	np		Severe	Spielmann et al. (1996)
1,2-Epoxycyclooctane	286-62-4	AP	10%	Solid		<2.5	4.5	3.1	Slight		Spielmann et al. (1996)
1,2-Epoxydodecane	2855-19-8	MD	10%	Solid		insoluble	n.s.	0	Nonirritant	Slight	Spielmann et al. (1996)
1,2-Epoxydodecane	2855-19-8	HO	10%	Solid		insoluble	n.s.	4.1	Slight		Spielmann et al. (1996)
Ethiosan		AP	10%	Unknown		5	8.5	3.8	Slight	Slight	Spielmann et al. (1996)
Ethiosan		WA	10%	Unknown		5	8.5	0	Nonirritant		Spielmann et al. (1996)
Ethyl butanal	97-96-1	HO	10%	Liquid		10	<7	3.6	Slight	Slight	Spielmann et al. (1996)
Ethyl butanal	97-96-1	WA	10%	Liquid		10	<7	0	Nonirritant		Spielmann et al. (1996)

Substance Name	CASRN	Test Lab	*In Vitro* Concentration Tested	*In Vitro* Physical Form Tested	Purity (%)	Solubility[1]	pH	IS(B)-10[2]	IS(B)-10 Classification	Overall IS(B)-10 Classification	Reference
Gadopentetic acid dimeglumine salt	86050-77-3	WA	10%	Unknown		soluble	n.s.	6.4	Severe	Severe	Spielmann et al. (1996)
Gadopentetic acid dimeglumine salt	86050-77-3	BG	10%	Unknown		soluble	n.s.	3	Severe		Spielmann et al. (1996)
Genomoll	115-96-8	HO	10%	Solid		5	6	9.2	Severe	Severe	Spielmann et al. (1996)
Genomoll	115-96-8	WA	10%	Solid		5	6	9.4	Severe		Spielmann et al. (1996)
C12/C14-Glucoside		BD	10%	Unknown		readily soluble	9	8.4	Moderate	Severe	Spielmann et al. (1996)
C12/C14-Glucoside		HK	10%	Unknown		readily soluble	9	10.1	Severe		Spielmann et al. (1996)
C12/C14-Glucoside		BG	10%	Unknown		readily soluble	9	10.2	Severe		Spielmann et al. (1996)
L-Glutamic acid hydrochloride	138-15-8	HO	10%	Unknown		490	0.9	14.2	Severe	Severe	Spielmann et al. (1996)
L-Glutamic acid hydrochloride	138-15-8	MD	10%	Unknown		490	0.9	11.7	Severe		Spielmann et al. (1996)
Glycediol		MD	10%	Unknown		insoluble	n.s.	0	Nonirritant	Slight	Spielmann et al. (1996)
Glycediol		HO	10%	Unknown		insoluble	n.s.	1.8	Slight		Spielmann et al. (1996)

Substance Name	CASRN	Test Lab	*In Vitro* Concentration Tested	*In Vitro* Physical Form Tested	Purity (%)	Solubility[1]	pH	IS(B)-10[2]	IS(B)-10 Classification	Overall IS(B)-10 Classification	Reference
Granuform	30525-89-4	BD	10%	Solid		250	4	2.9	Slight	Slight	Spielmann et al. (1996)
Granuform	30525-89-4	HO	10%	Solid		250	4	0	Nonirritant		Spielmann et al. (1996)
Hexahydrofarnesylacetone	502-69-2	BG	10%	Unknown		poorly soluble	n.s.	2.3	Slight	Slight	Spielmann et al. (1996)
Hexahydrofarnesylacetone	502-69-2	BD	10%	Unknown		poorly soluble	n.s.	1.2	Slight		Spielmann et al. (1996)
Hexamethylenetetramine	100-97-0	WA	10%	Unknown		874	8.5	5.8	Moderate	Moderate	Spielmann et al. (1996)
Hexamethylenetetramine	100-97-0	MD	10%	Unknown		874	8.5	4.3	Slight		Spielmann et al. (1996)
1,2,6-Hexanetriol	106-69-4	HK	10%	Solid		n.s.	4.5	11.5	Severe	Severe	Spielmann et al. (1996)
1,2,6-Hexanetriol	106-69-4	HO	10%	Solid		n.s.	4.5	4.3	Slight		Spielmann et al. (1996)
Hnol		AP	10%	Unknown		insoluble	n.s.	0.8	Nonirritant	Nonirritant	Spielmann et al. (1996)
Hnol		WA	10%	Unknown		insoluble	n.s.	0	Nonirritant		Spielmann et al. (1996)
Hoe MBF		BD	10%	Unknown		100	4.3	0	Nonirritant	Nonirritant	Spielmann et al. (1996)
Hoe MBF		MD	10%	Unknown		100	4.3	0	Nonirritant		Spielmann et al. (1996)

Substance Name	CASRN	Test Lab	*In Vitro* Concentration Tested	*In Vitro* Physical Form Tested	Purity (%)	Solubility[1]	pH	IS(B)-10[2]	IS(B)-10 Classification	Overall IS(B)-10 Classification	Reference
Hydo 98		BD	10%	Unknown		soluble	6.5	10.4	Severe	Severe	Spielmann et al. (1996)
Hydo 98		MD	10%	Unknown		soluble	6.5	12.9	Severe		Spielmann et al. (1996)
2-Hydroxyethyl imino disodium acetate	135-37-5	AP	10%	Unknown		n.s.	10.6	13.4	Severe	Severe	Spielmann et al. (1996)
2-Hydroxyethyl imino disodium acetate	135-37-5	HO	10%	Unknown		n.s.	10.6	8.9	Moderate		Spielmann et al. (1996)
2-Hydroxyisobutyric acid	594-61-6	BD	10%	Solid		1900	1	10.8	Severe	Severe	Spielmann et al. (1996)
2-Hydroxyisobutyric acid	594-61-6	WA	10%	Solid		1900	1	14.9	Severe		Spielmann et al. (1996)
Hypo 20		BG	10%	Unknown		readily soluble	6.5	7.2	Moderate	Moderate	Spielmann et al. (1996)
Hypo 20		HO	10%	Unknown		readily soluble	6.5	0	Nonirritant		Spielmann et al. (1996)
Hypo 36		AP	10%	Unknown		readily soluble	7	4	Severe	Severe	Spielmann et al. (1996)
Hypo 36		WA	10%	Unknown		readily soluble	7	4.2	Severe		Spielmann et al. (1996)

Substance Name	CASRN	Test Lab	*In Vitro* Concentration Tested	*In Vitro* Physical Form Tested	Purity (%)	Solubility[1]	pH	IS(B)-10[2]	IS(B)-10 Classification	Overall IS(B)-10 Classification	Reference
Hypo 45		BD	10%	Unknown		readily soluble	7	11.1	Severe	Slight	Spielmann et al. (1996)
Hypo 45		WA	10%	Unknown		readily soluble	7	2.5	Slight		Spielmann et al. (1996)
Hypo 45		BG	10%	Unknown		readily soluble	7	1.9	Slight		Spielmann et al. (1996)
Hypo 54		BG	10%	Unknown		soluble	6.5	4.3	Slight	Slight	Spielmann et al. (1996)
Hypo 54		HO	10%	Unknown		soluble	6.5	4	Slight		Spielmann et al. (1996)
Hyton		AP	10%	Unknown		soluble	8.5	17	Severe	Severe	Spielmann et al. (1996)
Hyton		BG	10%	Unknown		soluble	8.5	13.5	Severe		Spielmann et al. (1996)
Iminodiacetic acid	142-73-4	AP	10%	Solid		42	2.3	15.6	Severe	Severe	Spielmann et al. (1996)
Iminodiacetic acid	142-73-4	BD	10%	Solid		42	2.3	0.75	Nonirritant		Spielmann et al. (1996)
Iminodiacetic acid	142-73-4	BG	10%	Solid		42	2.3	8.4	Moderate		Spielmann et al. (1996)
Isobornyl acetate	125-12-2	HO	10%	Solid		< 1	n.s.	4.1	Slight	Slight	Spielmann et al. (1996)
Isobornyl acetate	125-12-2	BD	10%	Solid		< 1	n.s.	1.7	Slight		Spielmann et al. (1996)

Substance Name	CASRN	Test Lab	*In Vitro* Concentration Tested	*In Vitro* Physical Form Tested	Purity (%)	Solubility[1]	pH	IS(B)-10[2]	IS(B)-10 Classification	Overall IS(B)-10 Classification	Reference
Isobutanal	78-84-2	WA	10%	Liquid		67	<7	2.1	Slight	Slight	Spielmann et al. (1996)
Isobutanal	78-84-2	HK	10%	Liquid		67	<7	0	Nonirritant		Spielmann et al. (1996)
Isodecylglucoside		AP	10%	Unknown		readily soluble	9	17.2	Severe	Severe	Spielmann et al. (1996)
Isodecylglucoside		HO	10%	Unknown		readily soluble	9	9.9	Severe		Spielmann et al. (1996)
Isononylaldehyde	35127-50-5	BG	10%	Liquid		0.1	<7	0	Nonirritant	Nonirritant	Spielmann et al. (1996)
Isononylaldehyde	35127-50-5	WA	10%	Liquid		0.1	<7	0	Nonirritant		Spielmann et al. (1996)
alpha-Ketoglutaric acid	328-50-7	AP	10%	Solid		1000	1.75	19.1	Severe	Severe	Spielmann et al. (1996)
alpha-Ketoglutaric acid	328-50-7	BG	10%	Solid		1000	1.75	18.8	Severe		Spielmann et al. (1996)
Lactic acid	79-33-4	PhI	10%	Unknown		readily soluble	2	17.6	Severe	Severe	Spielmann et al. (1996)
alpha-Lactid	4511-42-6	AP	10%	Solid		soluble	3	13.5	Severe	Severe	Spielmann et al. (1996)
alpha-Lactid	4511-42-6	BG	10%	Solid		soluble	3	1.8	Slight		Spielmann et al. (1996)
alpha-Lactid	4511-42-6	BG	10%	Solid		soluble	3	10.5	Severe		Spielmann et al. (1996)
L-Lysine Monohydrate	39665-12-8	BD	10%	Solid		1500	10	10	Severe	Severe	Spielmann et al. (1996)
L-Lysine Monohydrate	39665-12-8	HO	10%	Solid		1500	10	8.25	Moderate		Spielmann et al. (1996)

Substance Name	CASRN	Test Lab	*In Vitro* Concentration Tested	*In Vitro* Physical Form Tested	Purity (%)	Solubility[1]	pH	IS(B)-10[2]	IS(B)-10 Classification	Overall IS(B)-10 Classification	Reference
Mecre		HK	10%	Unknown		mixable	7	n.p.			Spielmann et al. (1996)
Mecre		MD	10%	Unknown		mixable	7	n.p.			Spielmann et al. (1996)
3-Mercapto-1,2,4-triazole	3179-31-5	HK	10%	Solid		85	4	18.3	Severe	Severe	Spielmann et al. (1996)
3-Mercapto-1,2,4-triazole	3179-31-5	MD	10%	Solid		85	4	4.3	Slight		Spielmann et al. (1996)
m-Methoxybenzaldehyde	591-31-1	MD	10%	Solid		poorly soluble	n.s.	4.1	Slight	Slight	Spielmann et al. (1996)
m-Methoxybenzaldehyde	591-31-1	BD	10%	Solid		poorly soluble	n.s.	2.2	Slight		Spielmann et al. (1996)
Methyl acetate	79-20-9	BD	10%	Liquid		250	7	4.4	Slight	Slight	Spielmann et al. (1996)
Methyl acetate	79-20-9	HO	10%	Liquid		250	7	4.3	Slight		Spielmann et al. (1996)
Methylpentynol	77-75-8	AP	10%	Liquid		soluble	n.s.	15.4	Severe	Severe	Spielmann et al. (1996)
Methylpentynol	77-75-8	BD	10%	Liquid		soluble	n.s.	12.3	Severe		Spielmann et al. (1996)
N-(2-methylphenyl)-Imidodi-carbonimidic diamide	93-69-6	AP	10%	Solid		40	11.5	17.1	Severe	Severe	Spielmann et al. (1996)
N-(2-methylphenyl)-Imidodi-carbonimidic diamide	93-69-6	MD	10%	Solid		40	11.5	17.7	Severe		Spielmann et al. (1996)
2-Methyl-1-propanol	78-83-1	HK	10%	Liquid		15	3	17.7	Severe	Severe	Spielmann et al. (1996)
2-Methyl-1-propanol	78-83-1	MD	10%	Liquid		15	3	17.9	Severe		Spielmann et al. (1996)
Methyltriglycol	112-35-6	BD	10%	Liquid		readily soluble	7	4.9	Slight	Severe	Spielmann et al. (1996)
Methyltriglycol	112-35-6	HO	10%	Liquid		readily soluble	7	4.1	Severe		Spielmann et al. (1996)

Substance Name	CASRN	Test Lab	*In Vitro* Concentration Tested	*In Vitro* Physical Form Tested	Purity (%)	Solubility[1]	pH	IS(B)-10[2]	IS(B)-10 Classification	Overall IS(B)-10 Classification	Reference
Methyltriglycol	112-35-6	AP	10%	Liquid		readily soluble	7	11	Severe	Severe	Spielmann et al. (1996)
Methyltriglycol	112-35-6	HO	10%	Liquid		readily soluble	7	3	Severe		Spielmann et al. (1996)
Napt		HO	10%	Unknown		1000	n.s.	4.3	Slight	Slight	Spielmann et al. (1996)
Napt		WA	10%	Unknown		1000	n.s.	1.9	Slight		Spielmann et al. (1996)
Nitro-bis-octylamide		BG	10%	Unknown		insoluble	n.s.	1.7	Slight	Slight	Spielmann et al. (1996)
Nitro-bis-octylamide		HK	10%	Unknown		insoluble	n.s.	0	Nonirritant		Spielmann et al. (1996)
Olak		HK	10%	Unknown		soluble	8.3	18.9	Severe	Severe	Spielmann et al. (1996)
Olak		MD	10%	Unknown		soluble	8.3	16.1	Severe		Spielmann et al. (1996)
Ölesulf		BD	10%	Unknown		soluble	8	16.9	Severe	Severe	Spielmann et al. (1996)
Ölesulf		HK	10%	Unknown		soluble	8	16.8	Severe		Spielmann et al. (1996)
Phenylephrine hydrochloride	61-76-7	AP	10%	Solid		1000	7	8.6	Moderate	Severe	Spielmann et al. (1996)
Phenylephrine hydrochloride	61-76-7	HK	10%	Solid		1000	7	11.1	Severe		Spielmann et al. (1996)
Phenylthiourea	103-85-5	AP	10%	Solid		1	5.5	4	Slight	Slight	Spielmann et al. (1996)
Phenylthiourea	103-85-5	BD	10%	Solid		1	5.5	0	Nonirritant		Spielmann et al. (1996)
Phosphonat A		AP	10%	Unknown		3.6	2.1	6.8	Moderate	Moderate	Spielmann et al. (1996)
Phosphonat A		BG	10%	Unknown		3.6	2.1	6.6	Moderate		Spielmann et al. (1996)

Substance Name	CASRN	Test Lab	*In Vitro* Concentration Tested	*In Vitro* Physical Form Tested	Purity (%)	Solubility[1]	pH	IS(B)-10[2]	IS(B)-10 Classification	Overall IS(B)-10 Classification	Reference
Acefyllin piperazinate	18833-13-1	HK	10%	Solid		625	5	18.5	Severe	Severe	Spielmann et al. (1996)
Acefyllin piperazinate	18833-13-1	WA	10%	Solid		625	5	0	Nonirritant		Spielmann et al. (1996)
Acefyllin piperazinate	18833-13-1	BG	10%	Solid		625	5	2.9	Slight		Spielmann et al. (1996)
PO 2		AP	10%	Unknown		insoluble	n.s.	4.3	Slight	Slight	Spielmann et al. (1996)
PO 2		WA	10%	Unknown		insoluble	n.s.	0	Nonirritant		Spielmann et al. (1996)
Polyethylene glycol butyl ether	9004-77-7	AP	10%	Liquid		1000	6	10.9	Severe	Severe	Spielmann et al. (1996)
Polyethylene glycol butyl ether	9004-77-7	WA	10%	Liquid		1000	6	15.7	Severe		Spielmann et al. (1996)
Polyethylene glycol dimethyl ether	24991-55-7	HO	10%	Unknown		readily soluble	7	4.1	Slight	Slight	Spielmann et al. (1996)
Polyethylene glycol dimethyl ether	24991-55-7	WA	10%	Unknown		readily soluble	7	0	Nonirritant		Spielmann et al. (1996)
Polyethylene glycol	25322-68-3	MD	10%	Unknown		750	n.s.	1	Slight	Slight	Spielmann et al. (1996)
Polyethylene glycol	25322-68-3	WA	10%	Unknown		750	n.s.	0	Nonirritant		Spielmann et al. (1996)
Polyhexamethylene guanidine		BD	10%	Unknown		soluble	7.1	9.2	Severe	Severe	Spielmann et al. (1996)
Polyhexamethylene guanidine		BG	10%	Unknown		soluble	7.1	11	Severe		Spielmann et al. (1996)
Polysolvan	7397-62-8	AP	10%	Liquid		80	7	16.5	Severe	Severe	Spielmann et al. (1996)
Polysolvan	7397-62-8	HO	10%	Liquid		80	7	15.8	Severe		Spielmann et al. (1996)

Substance Name	CASRN	Test Lab	*In Vitro* Concentration Tested	*In Vitro* Physical Form Tested	Purity (%)	Solubility[1]	pH	IS(B)-10[2]	IS(B)-10 Classification	Overall IS(B)-10 Classification	Reference
Potassium cyanate	590-28-3	AP	10%	Solid		750	10	18.8	Severe	Severe	Spielmann et al. (1996)
Potassium cyanate	590-28-3	MD	10%	Solid		750	10	15.8	Severe		Spielmann et al. (1996)
Potassium hexacyanoferrate II	14459-95-1	HK	10%	Solid		250	9.5	17.8	Severe	Severe	Spielmann et al. (1996)
Potassium hexacyanoferrate II	14459-95-1	HO	10%	Solid		250	9.5	15.2	Severe		Spielmann et al. (1996)
Potassium hexacyanoferrate III	13756-66-2	BD	10%	Solid		310	8	4.2	Slight	Moderate	Spielmann et al. (1996)
Potassium hexacyanoferrate III	13756-66-2	MD	10%	Solid		310	8	6.25	Moderate		Spielmann et al. (1996)
2-Pseudojonon		HK	10%	Unknown		0.1	n.s.	8.7	Moderate	Moderate	Spielmann et al. (1996)
2-Pseudojonon		BG	10%	Unknown		0.1	n.s.	2.8	Slight		Spielmann et al. (1996)
RK Blau		HK	10%	Unknown		100	2.6	4	Slight	Slight	Spielmann et al. (1996)
RK Blau		MD	10%	Unknown		100	2.6	0	Nonirritant		Spielmann et al. (1996)
Rubinrot Y		AP	10%	Unknown		172		n.p.		Slight	Spielmann et al. (1996)
Rubinrot Y		HO	10%	Unknown		172		4	Slight		Spielmann et al. (1996)
Sacyclo		HO	10%	Unknown		insoluble	n.s.	3.4	Slight	Slight	Spielmann et al. (1996)
Sacyclo		MD	10%	Unknown		insoluble	n.s.	0	Nonirritant		Spielmann et al. (1996)
Sept		BD	10%	Unknown		soluble	3	4	Severe	Severe	Spielmann et al. (1996)
Sept		HK	10%	Unknown		soluble	3	10	Severe		Spielmann et al. (1996)

Substance Name	CASRN	Test Lab	*In Vitro* Concentration Tested	*In Vitro* Physical Form Tested	Purity (%)	Solubility[1]	pH	IS(B)-10[2]	IS(B)-10 Classification	Overall IS(B)-10 Classification	Reference
Surfactant Based Formulation 1-HZA			10%	Solution					Severe	Severe	Gettings et al. (1996)
Surfactant Based Formulation 2-HZB			10%	Solution					Moderate	Moderate	Gettings et al. (1996)
Surfactant Based Formulation 3-HZC			10%	Solution					Severe	Severe	Gettings et al. (1996)
Surfactant Based Formulation 4-HZD			10%	Solution					Moderate	Moderate	Gettings et al. (1996)
Surfactant Based Formulation 5-HZE			10%	Solution					Severe	Severe	Gettings et al. (1996)
Surfactant Based Formulation 6-HZF			10%	Solution					Severe	Severe	Gettings et al. (1996)
Surfactant Based Formulation 7-HZG			10%	Solution					Moderate	Moderate	Gettings et al. (1996)
Surfactant Based Formulation 8-HZH			10%	Solution					Slight	Slight	Gettings et al. (1996)
Surfactant Based Formulation 9-HZI			10%	Solution					Severe	Severe	Gettings et al. (1996)
Surfactant Based Formulation 10-HZJ			10%	Solution					Moderate	Moderate	Gettings et al. (1996)
Surfactant Based Formulation 11-HZK			10%	Solution					Severe	Severe	Gettings et al. (1996)
Surfactant Based Formulation 12-HZL			10%	Solution					Severe	Severe	Gettings et al. (1996)
Surfactant Based Formulation 13-HZM			10%	Solution					Slight	Slight	Gettings et al. (1996)
Surfactant Based Formulation 14-HZN			10%	Solution					Moderate	Moderate	Gettings et al. (1996)
Surfactant Based Formulation 15-HZP			10%	Solution					Slight	Slight	Gettings et al. (1996)
Surfactant Based Formulation 16-HZQ			10%	Solution					Slight	Slight	Gettings et al. (1996)

Substance Name	CASRN	Test Lab	*In Vitro* Concentration Tested	*In Vitro* Physical Form Tested	Purity (%)	Solubility[1]	pH	IS(B)-10[2]	IS(B)-10 Classification	Overall IS(B)-10 Classification	Reference
Surfactant Based Formulation 17-HZR			10%	Solution					Moderate	Moderate	Gettings et al. (1996)
Surfactant Based Formulation 18-HZS			10%	Solution					Severe	Severe	Gettings et al. (1996)
Surfactant Based Formulation 19-HZT			10%	Solution					Slight	Slight	Gettings et al. (1996)
Surfactant Based Formulation 20-HZU			10%	Solution					Moderate	Moderate	Gettings et al. (1996)
Surfactant Based Formulation 21-HZV			10%	Solution					Moderate	Moderate	Gettings et al. (1996)
Surfactant Based Formulation 22-HZW			10%	Solution					Moderate	Moderate	Gettings et al. (1996)
Surfactant Based Formulation 23-HZX			10%	Solution					Severe	Severe	Gettings et al. (1996)
Surfactant Based Formulation 24-HZY			10%	Solution					Severe	Severe	Gettings et al. (1996)
Surfactant Based Formulation 25-HZZ			10%	Solution					Slight	Slight	Gettings et al. (1996)
Trimethoxypropylsilane	1067-25-0	BD	10%	Liquid		poorly soluble	n.s.	3.7	Slight	Slight	Spielmann et al. (1996)
Trimethoxypropylsilane	1067-25-0	AP	10%	Liquid		poorly soluble	n.s.	3.9	Slight		Spielmann et al. (1996)
Trimethoxyoctylsilane	3069-40-7	HO	10%	Liquid		insoluble	n.s.	7.9	Moderate	Moderate	Spielmann et al. (1996)
Trimethoxyoctylsilane	3069-40-7	BG	10%	Liquid		insoluble	n.s.	2.1	Slight		Spielmann et al. (1996)
Silan 165	29055-11-6	HO	10%	Unknown		insoluble	n.s.	0.7	Nonirritant	Nonirritant	Spielmann et al. (1996)
Silan 165	29055-11-6	WA	10%	Unknown		insoluble	n.s.	0	Nonirritant		Spielmann et al. (1996)

Substance Name	CASRN	Test Lab	*In Vitro* Concentration Tested	*In Vitro* Physical Form Tested	Purity (%)	Solubility[1]	pH	IS(B)-10[2]	IS(B)-10 Classification	Overall IS(B)-10 Classification	Reference
Silan 167	41453-78-5	WA	10%	Unknown		soluble	n.s.	2.7	Slight	Slight	Spielmann et al. (1996)
Silan 167	41453-78-5	HO	10%	Unknown		soluble	n.s.	0.1	Nonirritant		Spielmann et al. (1996)
Silan 253	18784-74-2	BD	10%	Unknown		insoluble	<7	3	Severe	Severe	Spielmann et al. (1996)
Silan 253	18784-74-2	MD	10%	Unknown		insoluble	<7	3	Severe		Spielmann et al. (1996)
Sodium bisulfite	7631-90-5	AP	10%	Solid		readily soluble	4.5	12.7	Severe	Severe	Spielmann et al. (1996)
Sodium bisulfite	7631-90-5	MD	10%	Solid		readily soluble	4.5	13.9	Severe		Spielmann et al. (1996)
Sodium sulfite	7757-83-7	AP	10%	Solid		250	10	13.2	Severe	Severe	Spielmann et al. (1996)
Sodium sulfite	7757-83-7	BG	10%	Solid		250	10	11.3	Severe		Spielmann et al. (1996)
Sodium cyanate	917-61-3	MD	10%	Solid		110	10.4	14.8	Severe	Severe	Spielmann et al. (1996)
Sodium cyanate	917-61-3	WA	10%	Solid		110	10.4	10.5	Severe		Spielmann et al. (1996)
Sodium disilicate	13870-28-5	BG	10%	Solid		3.5	11.4	19.7	Severe	Severe	Spielmann et al. (1996)
Sodium disilicate	13870-28-5	HK	10%	Solid		3.5	11.4	20.7	Severe		Spielmann et al. (1996)
Sodium hydrogen sulfate	7681-38-1	HK	10%	Solid		1080	1.1	18.8	Severe	Severe	Spielmann et al. (1996)
Sodium hydrogen sulfate	7681-38-1	WA	10%	Solid		1080	1.1	16.7	Severe		Spielmann et al. (1996)
Sodium lauryl ether sulfate	3088-31-1	BG	10%	Unknown		soluble	8	10.5	Severe	Severe	Spielmann et al. (1996)
Sodium lauryl ether sulfate	3088-31-1	MD	10%	Unknown		soluble	8	17.7	Severe		Spielmann et al. (1996)

Substance Name	CASRN	Test Lab	*In Vitro* Concentration Tested	*In Vitro* Physical Form Tested	Purity (%)	Solubility[1]	pH	IS(B)-10[2]	IS(B)-10 Classification	Overall IS(B)-10 Classification	Reference
Sodium monochloroacetate	3926-62-3	HO	10%	Solid		440	4.5	7.5	Moderate	Moderate	Spielmann et al. (1996)
Sodium monochloroacetate	3926-62-3	BD	10%	Solid		440	4.5	0	Nonirritant		Spielmann et al. (1996)
Sodiumpyrosulfite	7681-57-4	AP	10%	Solid		650	4.6	17.4	Severe	Severe	Spielmann et al. (1996)
Sodiumpyrosulfite	7681-57-4	BD	10%	Solid		650	4.6	12.6	Severe		Spielmann et al. (1996)
Sodiumpyrosulfite	7681-57-4	bg	10%	Solid		650	4.6	14.6	Severe		Spielmann et al. (1996)
4-((2-sulfatoethyl)sulfonyl)-aniline	2494-89-5	AP	10%	Unknown		soluble	7	18	Severe	Severe	Spielmann et al. (1996)
4-((2-sulfatoethyl)sulfonyl)-aniline	2494-89-5	HK	10%	Unknown		soluble	7	20.1	Severe		Spielmann et al. (1996)
TA 01946 Alkylsilan		AP	10%	Unknown		0.014	n.s.	7.6	Moderate	Severe	Spielmann et al. (1996)
TA 01946 Alkylsilan		HK	10%	Unknown		0.014	n.s.	10	Severe		Spielmann et al. (1996)
Theophylline sodium acetate	8002-89-9	AP	10%	Unknown		50	11	13.4	Severe	Severe	Spielmann et al. (1996)
Theophylline sodium acetate	8002-89-9	HO	10%	Unknown		50	11	5.4	Moderate		Spielmann et al. (1996)
Tocla		BD	10%	Unknown		40	6	12.9	Severe	Severe	Spielmann et al. (1996)
Tocla		HK	10%	Unknown		40	6	19.7	Severe		Spielmann et al. (1996)
Triisooctylamine	25549-16-0	BG	10%	Solid		0.5	7	0.8	Nonirritant	Nonirritant	Spielmann et al. (1996)
Triisooctylamine	25549-16-0	MD	10%	Solid		0.5	7	0	Nonirritant		Spielmann et al. (1996)

Substance Name	CASRN	Test Lab	*In Vitro* Concentration Tested	*In Vitro* Physical Form Tested	Purity (%)	Solubility[1]	pH	IS(B)-10[2]	IS(B)-10 Classification	Overall IS(B)-10 Classification	Reference
2,2,3-Trimethyl-3-Cyclo-pentene-1-acetaldehyde	4501-58-0	BG	10%	Solid		< 2.5	2.3	2.9	Slight	Slight	Spielmann et al. (1996)
2,2,3-Trimethyl-3-Cyclo-pentene-1-acetaldehyde	4501-58-0	AP	10%	Solid		< 2.5	2.3	2.3	Slight		Spielmann et al. (1996)
Trioxane	110-88-3	HK	10%	Solid		172	n.s.	9.25	Severe	Severe	Spielmann et al. (1996)
Trioxane	110-88-3	WA	10%	Solid		172	n.s.	13.4	Severe		Spielmann et al. (1996)
Wessalith Slurry		BG	10%	Unknown		readily soluble	11	3.13	Slight	Severe	Spielmann et al. (1996)
Wessalith Slurry		WA	10%	Unknown		readily soluble	11	10	Severe		Spielmann et al. (1996)
Xanthinol nicotinate	437-74-1	WA	10%	Solid		250	6	4	Slight	Severe	Spielmann et al. (1996)
Xanthinol nicotinate	437-74-1	HK	10%	Solid		250	6	11.3	Severe		Spielmann et al. (1996)

Abbreviation: CASRN: Chemical Abstracts Service Registy Number.

[1] Solubility = obtained from literature references; where available, expressed as g/mL

[2] IS(B)-10 represents irritation scores that were calculated using a method similar to the one described in Kalweit et al. (1987) where the *in vitro* score was obtained using a 10% concentration and where *in vivo* results were obtained at 100% concentration.

Appendix C8

Data Sorted by Substance for IS(B)-100 Analysis Method

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Substance Name	CASRN	Test Lab	Concentration Tested	Physical Form Tested	Purity (%)	Solubility[1]	pH	IS(B)-100[2]	IS(B)-100 Classification	Overall IS(B)-100 Classification	Reference
Acetone	67-64-1		100%					15.32	Severe	Severe	Gilleron et al. (1997)
7-Acetoxyheptanal		MD	100%	Unknown		insoluble		4.9	Slight	Severe	Spielmann et al. (1996)
7-Acetoxyheptanal		WA	100%	Unknown		insoluble		17	Severe		Spielmann et al. (1996)
n-Acetyl-Methionine	1115-47-5	MD	100%	Solid		83	2.2	n.p.		Severe	Spielmann et al. (1996)
n-Acetyl-Methionine	1115-47-5	WA	100%	Solid		83	2.2	10.6	Severe		Spielmann et al. (1996)
Allyl alcohol	107-18-6		100%					12.4	Severe	Severe	Gilleron et al. (1996)
Ambuphylline	5634-34-4	BG	100%	Solid		600	9	12.8	Severe	Severe	Spielmann et al. (1996)
Ambuphylline	5634-34-4	MD	100%	Solid		600	9	16.9	Severe		Spielmann et al. (1996)
4-Amino-5-methoxy-2-methylbenzenesulfonic acid	6471-78-9	AP	100%	Unknown		3	1.5	14.4	Severe	Severe	Spielmann et al. (1996)
4-Amino-5-methoxy-2-methylbenzenesulfonic acid	6471-78-9	WA	100%	Unknown		3	1.5	13.6	Severe		Spielmann et al. (1996)
4-Amino-5-methoxy-2-methylbenzenesulfonic acid	6471-78-9	BG	100%	Unknown		3	1.5	8.5	Moderate		Spielmann et al. (1996)
2-Aminophemol	95-55-6		100%					0.8	Nonirritant	Nonirritant	Gilleron et al. (1996)
Ammonium nitrate	6484-52-2		100%					15.34	Severe	Severe	Gilleron et al. (1997)

Substance Name	CASRN	Test Lab	Concentration Tested	Physical Form Tested	Purity (%)	Solubility[1]	pH	IS(B)-100[2]	IS(B)-100 Classification	Overall IS(B)-100 Classification	Reference
Ammonium persulfate	7727-54-0	HO	100%	Solid		560	1.5	n.p.			Spielmann et al. (1996)
Ammonium persulfate	7727-54-0	WA	100%	Solid		560	1.5	n.p.			Spielmann et al. (1996)
Anisole	100-66-3	AP	100%	Liquid		insoluble		19.1	Severe	Severe	Spielmann et al. (1996)
Anisole	100-66-3	HK	100%	Liquid		insoluble		18.5	Severe		Spielmann et al. (1996)
Anthracene	120-12-7		100%					0	Nonirritant	Nonirritant	Gilleron et al. (1996)
L-Aspartic acid	70-47-3		100%					1.06	Slight	Slight	Gilleron et al. (1997)
B 25		BG	100%	Unknown		insoluble		0	Nonirritant	Nonirritant	Spielmann et al. (1996)
B 25		WA	100%	Unknown		insoluble		0	Nonirritant		Spielmann et al. (1996)
Benzethonium chloride	121-54-0		100%					15.4	Severe	Severe	Gilleron et al. (1996)
n-Butanal	123-72-8	HK	100%	Liquid		71	<7	20.3	Severe	Severe	Spielmann et al. (1996)
n-Butanal	123-72-8	HO	100%	Liquid		71	<7	18.1	Severe		Spielmann et al. (1996)
n-Butanol	71-36-3	BD	100%	Liquid		79	7	13	Severe	Severe	Spielmann et al. (1996)
n-Butanol	71-36-3	HK	100%	Liquid		79	7	20.2	Severe		Spielmann et al. (1996)

Substance Name	CASRN	Test Lab	Concentration Tested	Physical Form Tested	Purity (%)	Solubility[1]	pH	IS(B)-100[2]	IS(B)-100 Classification	Overall IS(B)-100 Classification	Reference
Butyl acetate	123-86-4		100%					17.21	Severe	Severe	Gilleron et al. (1997)
Butyl carbamate	592-35-8	BD	100%	Solid		1		11.5	Severe	Severe	Spielmann et al. (1996)
Butyl carbamate	592-35-8	MD	100%	Solid		1		11.6	Severe		Spielmann et al. (1996)
Butyl carbamate	592-35-8	BG	100%	Solid		1		14.9	Severe		Spielmann et al. (1996)
Caffeine sodium benzoate	8000-95-1	BD	100%	Solid		500	7	7.4	Moderate	Severe	Spielmann et al. (1996)
Caffeine sodium benzoate	8000-95-1	WA	100%	Solid		500	7	17.9	Severe		Spielmann et al. (1996)
Caffeine sodium benzoate	8000-95-1	BG	100%	Solid		500	7	14	Severe		Spielmann et al. (1996)
Caffeine sodium salicylate	8002-85-5	BG	100%	Solid		400	7	16	Severe	Severe	Spielmann et al. (1996)
Caffeine sodium salicylate	8002-85-5	WA	100%	Solid		400	7	18.8	Severe		Spielmann et al. (1996)
Camphen	79-92-5	BG	100%	Solid		insoluble	7	4	Slight	Slight	Spielmann et al. (1996)
Camphen	79-92-5	HK	100%	Solid		insoluble	7	n.p.			Spielmann et al. (1996)
Captan 90 concentrate	133-06-2		100%					15.07	Severe	Severe	Gilleron et al. (1997)
4-Carboxybenzaldehyde	619-66-9		100%					3.95	Slight	Slight	Gilleron et al. (1997)

Substance Name	CASRN	Test Lab	Concentration Tested	Physical Form Tested	Purity (%)	Solubility[1]	pH	IS(B)-100[2]	IS(B)-100 Classification	Overall IS(B)-100 Classification	Reference
Cerium-2-ethylhexanoate	24593-34-8	BG	100%	Unknown		n.s.	3	15.1	Severe	Severe	Spielmann et al. (1996)
Cerium-2-ethylhexanoate	24593-34-8	WA	100%	Unknown		n.s.	3	19.25	Severe		Spielmann et al. (1996)
Chlorhexidine	55-56-1		100%					14.87	Severe	Severe	Gilleron et al. (1997)
1-Chloroctane-8-ol		AP	100%	Unknown		insoluble		18.7	Severe	Severe	Spielmann et al. (1996)
1-Chloroctane-8-ol		MD	100%	Unknown		insoluble		14.3	Severe		Spielmann et al. (1996)
Cyclohexanol	108-93-0		100%					18.96	Severe	Severe	Gilleron et al. (1997)
Cyclohexanone	108-94-1		100%					14.5	Severe	Severe	Gilleron et al. (1996)
3-Cyclohexene-1-methanol	1679-51-2	BG	100%	Unknown		insoluble		18.9	Severe	Severe	Spielmann et al. (1996)
3-Cyclohexene-1-methanol	1679-51-2	HO	100%	Unknown		insoluble		19	Severe		Spielmann et al. (1996)
DC 8		BG	100%	Unknown		insoluble		0	Nonirritant	Moderate	Spielmann et al. (1996)
DC 8		WA	100%	Unknown		insoluble		5	Moderate		Spielmann et al. (1996)
Deoxycholic acid, sodium salt	302-95-4		100%					9.7	Severe	Severe	Gilleron et al. (1996)
Diacetone alcohol	123-42-2		100%					15.1	Severe	Severe	Gilleron et al. (1996)

Substance Name	CASRN	Test Lab	Concentration Tested	Physical Form Tested	Purity (%)	Solubility[1]	pH	IS(B)-100[2]	IS(B)-100 Classification	Overall IS(B)-100 Classification	Reference
Dibenzoyl-L-tartaric acid	2743-38-6		100%					13.34	Severe	Severe	Gilleron et al. (1997)
Dibenzoyl-L-tartaric acid	2743-38-6		100%					4.2	Slight		Gilleron et al. (1996)
Dibenzyl phosphate	1623-08-1		100%					15.16	Severe	Severe	Gilleron et al. (1997)
1,4-Dibutoxy-benzene	104-36-9	HO	100%	Unknown		0.2	7	0	Nonirritant	Nonirritant	Spielmann et al. (1996)
1,4-Dibutoxy-benzene	104-36-9	WA	100%	Unknown		0.2	7	n.p.			Spielmann et al. (1996)
2,6-Dichlorobenzoyl chloride	4659-45-4		100%					10.74	Severe	Severe	Gilleron et al. (1997)
2,4-Dicholor-5-sulfamolyl-benzoic acid	2736-23-4		100%					3.8	Slight	Slight	Gilleron et al. (1996)
Diepoxid 126	2386-87-0	AP	100%	Liquid		insoluble		10	Severe	Severe	Spielmann et al. (1996)
Diepoxid 126	2386-87-0	MD	100%	Liquid		insoluble		15.6	Severe		Spielmann et al. (1996)
Diepoxid 126	2386-87-0	BG	100%	Liquid		insoluble		6	Moderate		Spielmann et al. (1996)
Dimethyl biguanidine	657-24-9		100%					8.4	Moderate	Moderate	Gilleron et al. (1996)
2,2-Dimethylbutanoic acid	595-37-9		100%					15.31	Severe	Severe	Gilleron et al. (1997)

Substance Name	CASRN	Test Lab	Concentration Tested	Physical Form Tested	Purity (%)	Solubility[1]	pH	IS(B)-100[2]	IS(B)-100 Classification	Overall IS(B)-100 Classification	Reference
2,5-Dimethylhexanediol	110-03-2		100%					15.33	Severe	Severe	Gilleron et al. (1997)
2,5-Dimethylhexanediol	110-03-2	HK	100%	Solid		n.s.		16.6	Severe		Spielmann et al. (1996)
2,5-Dimethylhexanediol	110-03-2	HO	100%	Solid		n.s.		11.1	Severe		Spielmann et al. (1996)
2,5-Dimethylhexanediol	110-03-2	BG	100%	Solid		n.s.					Spielmann et al. (1996)
3,6-Dimethyloctanol		BG	100%	Unknown		poorly soluble	7	4.3	Slight	Slight	Spielmann et al. (1996)
3,6-Dimethyloctanol		BD	100%	Unknown		poorly soluble	7	4.3	Slight		Spielmann et al. (1996)
4,4-Dimethyl-3-oxo-pentanenitrile	59997-51-2	AP	100%	Solid		0.6		6.7	Moderate	Moderate	Spielmann et al. (1996)
4,4-Dimethyl-3-oxo-pentanenitrile	59997-51-2	WA	100%	Solid		0.6		5.7	Moderate		Spielmann et al. (1996)
1-(2,6-dimethylphenoxy)-2-propanone	53012-41-2	HK	100%	Liquid		insoluble	5	19.3	Severe	Severe	Spielmann et al. (1996)
1-(2,6-dimethylphenoxy)-2-propanone	53012-41-2	WA	100%	Liquid		insoluble	5	12	Severe		Spielmann et al. (1996)
1-(2,6-dimethylphenoxy)-2-propanone	53012-41-2	BG	100%	Liquid		insoluble	5	4.1	Slight		Spielmann et al. (1996)
Dimethyl sulfoxide	67-68-5		100%					11.3	Severe	Severe	Gilleron et al. (1996)

Substance Name	CASRN	Test Lab	Concentration Tested	Physical Form Tested	Purity (%)	Solubility[1]	pH	IS(B)-100[2]	IS(B)-100 Classification	Overall IS(B)-100 Classification	Reference
Diphocars		HK	100%	Unknown		soluble		17.9	Severe	Severe	Spielmann et al. (1996)
Diphocars		HO	100%	Unknown		soluble		12.3	Severe		Spielmann et al. (1996)
1,2-Dodecanediol	1119-87-5	AP	100%	Solid		insoluble		2.3	Slight	Slight	Spielmann et al. (1996)
1,2-Dodecanediol	1119-87-5	BG	100%	Solid		insoluble		4.1	Slight		Spielmann et al. (1996)
1,2-Dodecanediol	1119-87-5	BG	100%	Solid		insoluble			Nonirritant		Spielmann et al. (1996)
DTPA Pentasodium salt	140-01-2	BG	100%	Unknown		readily soluble	11.5	19.4	Severe	Severe	Spielmann et al. (1996)
DTPA Pentasodium salt	140-01-2	WA	100%	Unknown		readily soluble	11.5	19.9	Severe		Spielmann et al. (1996)
Ede 140		WA	100%	Unknown		insoluble		0	Nonirritant	Slight	Spielmann et al. (1996)
Ede 140		BD	100%	Unknown		insoluble		4.6	Slight		Spielmann et al. (1996)
EDTA dipotassium	25105-12-9		100%					0	Nonirritant	Nonirritant	Gilleron et al. (1996)
1,2-Epoxycyclooctane	286-62-4	MD	100%	Solid		<2.5	4.5	n.p.		Moderate	Spielmann et al. (1996)
1,2-Epoxycyclooctane	286-62-4	AP	100%	Solid		<2.5	4.5	7	Moderate		Spielmann et al. (1996)

Substance Name	CASRN	Test Lab	Concentration Tested	Physical Form Tested	Purity (%)	Solubility[1]	pH	IS(B)-100[2]	IS(B)-100 Classification	Overall IS(B)-100 Classification	Reference
1,2-Epoxydodecane	2855-19-8	MD	100%	Solid		insoluble		1.4	Slight	Moderate	Spielmann et al. (1996)
1,2-Epoxydodecane	2855-19-8	HO	100%	Solid		insoluble		8.5	Moderate		Spielmann et al. (1996)
Ethanol	64-17-5		100%					11.3	Severe	Severe	Gilleron et al. (1996)
Ethanol	64-17-5		100%					14.97	Severe		Gilleron et al. (1997)
Ethiosan		AP	100%	Unknown		5	8.5	n.p.			Spielmann et al. (1996)
Ethiosan		WA	100%	Unknown		5	8.5	n.p.			Spielmann et al. (1996)
2-Ethoxyethanol	110-80-5		100%					10.5	Severe	Severe	Gilleron et al. (1996)
Ethyl acetate	141-78-6		100%					19.32	Severe	Severe	Gilleron et al. (1997)
Ethylacetoacetate	141-97-9		100%					10	Severe	Severe	Gilleron et al. (1996)
Ethyl butanal	97-96-1	HO	100%	Liquid		10	<7	17.4	Severe	Severe	Spielmann et al. (1996)
Ethyl butanal	97-96-1	WA	100%	Liquid		10	<7	18.7	Severe		Spielmann et al. (1996)
2-Ethyl-1-hexanol	104-76-7		100%					12.71	Severe	Severe	Gilleron et al. (1997)
Ethyl-2-methylacetoacetate	609-14-3		100%					12.94	Severe	Severe	Gilleron et al. (1997)
Ethyl trimethyl acetate	3938-95-2		100%					13.82	Severe	Severe	Gilleron et al. (1997)

Substance Name	CASRN	Test Lab	Concentration Tested	Physical Form Tested	Purity (%)	Solubility[1]	pH	IS(B)-100[2]	IS(B)-100 Classification	Overall IS(B)-100 Classification	Reference
Fomesafen	72128-02-0		100%					1.21	Slight	Slight	Gilleron et al. (1997)
Furan	110-00-9		100%					5.5	Moderate	Moderate	Gilleron et al. (1996)
Gadopentetic acid dimeglumine salt	86050-77-3	WA	100%	Unknown		soluble		8.2	Moderate	Moderate	Spielmann et al. (1996)
Gadopentetic acid dimeglumine salt	86050-77-3	BG	100%	Unknown		soluble		3.2	Slight		Spielmann et al. (1996)
Gamma-butyrolactone	96-48-0		100%					13.9	Severe	Severe	Gilleron et al. (1996)
Gamma-butyrolactone	96-48-0		100%					19.39	Severe		Gilleron et al. (1997)
Genomoll	115-96-8	HO	100%	Solid		5	6	11.6	Severe	Severe	Spielmann et al. (1996)
Genomoll	115-96-8	WA	100%	Solid		5	6	9.9	Severe		Spielmann et al. (1996)
Gluconolactone	90-80-2		100%					4.6	Slight	Slight	Gilleron et al. (1996)
C12/C14-Glucoside		BD	100%	Unknown		readily soluble	9	16.7	Severe	Severe	Spielmann et al. (1996)
C12/C14-Glucoside		HK	100%	Unknown		readily soluble	9	16.3	Severe		Spielmann et al. (1996)
C12/C14-Glucoside		BG	100%	Unknown		readily soluble	9	16.5	Severe		Spielmann et al. (1996)
DL-Glutamic acid	19285-83-7		100%					0.7	Nonirritant	Nonirritant	Gilleron et al. (1996)

Substance Name	CASRN	Test Lab	Concentration Tested	Physical Form Tested	Purity (%)	Solubility[1]	pH	IS(B)-100[2]	IS(B)-100 Classification	Overall IS(B)-100 Classification	Reference
L-Glutamic acid hydrochloride	138-15-8	HO	100%	Unknown		490	0.9	11.7	Severe	Severe	Spielmann et al. (1996)
L-Glutamic acid hydrochloride	138-15-8	MD	100%	Unknown		490	0.9	15.2	Severe		Spielmann et al. (1996)
Glycediol		MD	100%	Unknown		insoluble		0.58	Nonirritant	Slight	Spielmann et al. (1996)
Glycediol		HO	100%	Unknown		insoluble		3.5	Slight		Spielmann et al. (1996)
Glycerol	56-81-5		100%					14.78	Severe	Severe	Gilleron et al. (1997)
3-Glycidopropyltrimethoxysilane	2530-83-8		100%					4.3	Slight	Slight	Gilleron et al. (1996)
Granuform	30525-89-4	BD	100%	Solid		250	4	0	Nonirritant	Nonirritant	Spielmann et al. (1996)
Granuform	30525-89-4	HO	100%	Solid		250	4	0	Nonirritant		Spielmann et al. (1996)
Hexadecyltrimethylammonium bromide	57-09-0		100%					10.8	Severe	Severe	Gilleron et al. (1996)
Hexahydrofarnesylacetone	502-69-2	BG	100%	Unknown		poorly soluble		8	Moderate	Moderate	Spielmann et al. (1996)
Hexahydrofarnesylacetone	502-69-2	BD	100%	Unknown		poorly soluble		4.2	Slight		Spielmann et al. (1996)
Hexamethylenetetramine	100-97-0	WA	100%	Unknown		874	8.5	11.1	Severe	Severe	Spielmann et al. (1996)
Hexamethylenetetramine	100-97-0	MD	100%	Unknown		874	8.5	11.2	Severe		Spielmann et al. (1996)

Substance Name	CASRN	Test Lab	Concentration Tested	Physical Form Tested	Purity (%)	Solubility[1]	pH	IS(B)-100[2]	IS(B)-100 Classification	Overall IS(B)-100 Classification	Reference
Hexane	110-54-3		100%					3.1	Slight	Slight	Gilleron et al. (1996)
1,2,6-Hexanetriol	106-69-4	HK	100%	Solid		n.s.	4.5	18.8	Severe	Severe	Spielmann et al. (1996)
1,2,6-Hexanetriol	106-69-4	HO	100%	Solid		n.s.	4.5	15.3	Severe		Spielmann et al. (1996)
Hexanol	111-27-3		100%					17.56	Severe	Severe	Gilleron et al. (1997)
Hnol		AP	100%	Unknown		insoluble		2.1	Slight	Moderate	Spielmann et al. (1996)
Hnol		WA	100%	Unknown		insoluble		6	Moderate		Spielmann et al. (1996)
Hoe MBF		BD	100%	Unknown		100	4.3	0	Nonirritant	Nonirritant	Spielmann et al. (1996)
Hoe MBF		MD	100%	Unknown		100	4.3	0.35	Nonirritant		Spielmann et al. (1996)
Hydo 98		BD	100%	Unknown		soluble	6.5	11.2	Severe	Severe	Spielmann et al. (1996)
Hydo 98		MD	100%	Unknown		soluble	6.5	n.p.			Spielmann et al. (1996)
Hydroalcoholic Formulation 1-5% Alcohol Containing Formulation			100%	Solution				4.6	Slight	Slight	Gettings et al. (1991)
Hydroalcoholic Formulation 2-10% Alcohol Containing			100%	Solution				5	Moderate	Moderate	Gettings et al. (1991)
Hydroalcoholic Formulation 3-15% Alcohol Containing			100%	Solution				8.5	Moderate	Moderate	Gettings et al. (1991)

Substance Name	CASRN	Test Lab	Concentration Tested	Physical Form Tested	Purity (%)	Solubility[1]	pH	IS(B)-100[2]	IS(B)-100 Classification	Overall IS(B)-100 Classification	Reference
Hydroalcoholic Formulation 4-20% Alcohol Containing			100%	Solution				5.3	Moderate	Moderate	Gettings et al. (1991)
Hydroalcoholic Formulation 5-33% Alcohol Containing Formulation (PROD-00184)			100%	Solution				n.p.	No Data	No Data	Gettings et al. (1991)
Hydroalcoholic Formulation 6-40% Alcohol Containing			100%	Solution				11.9	Severe	Severe	Gettings et al. (1991)
Hydroalcoholic Formulation 7-55% Alcohol Containing			100%	Solution				12.8	Severe	Severe	Gettings et al. (1991)
Hydroalcoholic Formulation 8-65% Alcohol Containing			100%	Solution				12.7	Severe	Severe	Gettings et al. (1991)
Hydroalcoholic Formulation 9-83% Alcohol Containing			100%	Solution				13.8	Severe	Severe	Gettings et al. (1991)
Hydroalcoholic Formulation 10-90% Alcohol Containing			100%	Solution				13.6	Severe	Severe	Gettings et al. (1991)
2-Hydroxyethyl imino disodium acetate	135-37-5	AP	100%	Unknown		n.s.	10.6	15.5	Severe	Severe	Spielmann et al. (1996)
2-Hydroxyethyl imino disodium acetate	135-37-5	HO	100%	Unknown		n.s.	10.6	11	Severe		Spielmann et al. (1996)
2-Hydroxyisobutyric acid	594-61-6	BD	100%	Solid		1900	1	11.3	Severe	Severe	Spielmann et al. (1996)
2-Hydroxyisobutyric acid	594-61-6	WA	100%	Solid		1900	1	15.6	Severe		Spielmann et al. (1996)

Substance Name	CASRN	Test Lab	Concentration Tested	Physical Form Tested	Purity (%)	Solubility[1]	pH	IS(B)-100[2]	IS(B)-100 Classification	Overall IS(B)-100 Classification	Reference
Hypo 20		BG	100%	Unknown		readily soluble	6.5	8.9	Moderate	Moderate	Spielmann et al. (1996)
Hypo 20		HO	100%	Unknown		readily soluble	6.5	4.12	Slight		Spielmann et al. (1996)
Hypo 36		AP	100%	Unknown		readily soluble	7	15.9	Severe	Severe	Spielmann et al. (1996)
Hypo 36		WA	100%	Unknown		readily soluble	7	10	Severe		Spielmann et al. (1996)
Hypo 45		BD	100%	Unknown		readily soluble	7	4.4	Slight	Severe	Spielmann et al. (1996)
Hypo 45		WA	100%	Unknown		readily soluble	7	8.7	Moderate		Spielmann et al. (1996)
Hypo 45		BG	100%	Unknown		readily soluble	7	11.9	Severe		Spielmann et al. (1996)
Hypo 54		BG	100%	Unknown		soluble	6.5	4.1	Slight	Slight	Spielmann et al. (1996)
Hypo 54		HO	100%	Unknown		soluble	6.5	4.2	Slight		Spielmann et al. (1996)
Hyton		AP	100%	Unknown		soluble	8.5	18.6	Severe	Severe	Spielmann et al. (1996)
Hyton		BG	100%	Unknown		soluble	8.5	18.2	Severe		Spielmann et al. (1996)
Imidazole	288-32-4		100%					18.7	Severe	Severe	Gilleron et al. (1996)
Imidazole	288-32-4		100%					19.43	Severe		Gilleron et al. (1997)

Substance Name	CASRN	Test Lab	Concentration Tested	Physical Form Tested	Purity (%)	Solubility[1]	pH	IS(B)-100[2]	IS(B)-100 Classification	Overall IS(B)-100 Classification	Reference
Iminodiacetic acid	142-73-4	AP	100%	Solid		42	2.3	12.8	Severe	Severe	Spielmann et al. (1996)
Iminodiacetic acid	142-73-4	BD	100%	Solid		42	2.3	0.85	Nonirritant		Spielmann et al. (1996)
Iminodiacetic acid	142-73-4	BG	100%	Solid		42	2.3	6.9	Moderate		Spielmann et al. (1996)
Iminodibenzyl	494-19-9		100%					0	Nonirritant	Nonirritant	Gilleron et al. (1996)
Isobornyl acetate	125-12-2	HO	100%	Solid		< 1		4.6	Slight	Moderate	Spielmann et al. (1996)
Isobornyl acetate	125-12-2	BD	100%	Solid		< 1		8.1	Moderate		Spielmann et al. (1996)
Isobutanal	78-84-2	WA	100%	Liquid		67	<7	19.4	Severe	Severe	Spielmann et al. (1996)
Isobutanal	78-84-2	HK	100%	Liquid		67	<7	20	Severe		Spielmann et al. (1996)
Isobutanol	78-83-1		100%					19.41	Severe	Severe	Gilleron et al. (1997)
Isodecylglucoside		AP	100%	Unknown		readily soluble	9	18	Severe	Severe	Spielmann et al. (1996)
Isodecylglucoside		HO	100%	Unknown		readily soluble	9	10.7	Severe		Spielmann et al. (1996)
Isononylaldehyde	35127-50-5	BG	100%	Liquid		0.1	<7	4.5	Slight	Severe	Spielmann et al. (1996)
Isononylaldehyde	35127-50-5	WA	100%	Liquid		0.1	<7	10	Severe		Spielmann et al. (1996)

Substance Name	CASRN	Test Lab	Concentration Tested	Physical Form Tested	Purity (%)	Solubility[1]	pH	IS(B)-100[2]	IS(B)-100 Classification	Overall IS(B)-100 Classification	Reference
Isopropanol	67-63-0		100%					14.8	Severe	Severe	Gilleron et al. (1997)
alpha-Ketoglutaric acid	328-50-7	AP	100%	Solid		1000	1.75	19.8	Severe	Severe	Spielmann et al. (1996)
alpha-Ketoglutaric acid	328-50-7	BG	100%	Solid		1000	1.75	19.7	Severe		Spielmann et al. (1996)
Lactic acid	79-33-4	PhI	100%	Unknown		readily soluble	2	19.6	Severe	Severe	Spielmann et al. (1996)
alpha-Lactid	4511-42-6	AP	100%	Solid		soluble	3	4	Slight	Slight	Spielmann et al. (1996)
alpha-Lactid	4511-42-6	BG	100%	Solid		soluble	3	1.1	Slight		Spielmann et al. (1996)
alpha-Lactid	4511-42-6	BG	100%	Solid		soluble	3	6.6	Moderate		Spielmann et al. (1996)
N-Lauroylsarcosine, sodium salt	7631-98-3		100%					12.7	Severe	Severe	Gilleron et al. (1996)
Laurylsulfobetaine	14933-08-5		100%					8.3	Moderate	Moderate	Gilleron et al. (1996)
L-Lysine Monohydrate	39665-12-8	BD	100%	Solid		1500	10	10.4	Severe	Severe	Spielmann et al. (1996)
L-Lysine Monohydrate	39665-12-8	HO	100%	Solid		1500	10	16.9	Severe		Spielmann et al. (1996)
Magnesium carbonate	56378-72-4		100%					1.4	Slight	Slight	Gilleron et al. (1996)
Maneb	12427-38-2		100%					0.16	Nonirritant	Nonirritant	Gilleron et al. (1997)
Mecre		HK	100%	Unknown		mixable	7	n.p.			Spielmann et al. (1996)
Mecre		MD	100%	Unknown		mixable	7	n.p.			Spielmann et al. (1996)
3-Mercapto-1,2,4-triazole	3179-31-5	HK	100%	Solid		85	4	n.p.			Spielmann et al. (1996)
3-Mercapto-1,2,4-triazole	3179-31-5	MD	100%	Solid		85	4	n.p.			Spielmann et al. (1996)

Substance Name	CASRN	Test Lab	Concentration Tested	Physical Form Tested	Purity (%)	Solubility[1]	pH	IS(B)-100[2]	IS(B)-100 Classification	Overall IS(B)-100 Classification	Reference
Methanol	67-56-1		100%					12.2	Severe	Severe	Gilleron et al. (1996)
m-Methoxybenzaldehyde	591-31-1	MD	100%	Solid		poorly soluble		13.7	Severe	Severe	Spielmann et al. (1996)
m-Methoxybenzaldehyde	591-31-1	BD	100%	Solid		poorly soluble		11.6	Severe		Spielmann et al. (1996)
2-Methoxyethanol	109-86-4		100%					14.5	Severe	Severe	Gilleron et al. (1996)
Methyl acetate	79-20-9	BD	100%	Liquid		250	7	19.8	Severe	Severe	Spielmann et al. (1996)
Methyl acetate	79-20-9	HO	100%	Liquid		250	7	16.1	Severe		Spielmann et al. (1996)
Methyl acetate	79-20-9		100%					18.98	Severe		Gilleron et al. (1997)
Methyl cyanoacetate	105-34-0		100%					16.31	Severe	Severe	Gilleron et al. (1997)
Methylcyclopentane	96-37-7		100%					17.17	Severe	Severe	Gilleron et al. (1997)
Methyl ethyl ketone	78-93-3		100%					18.35	Severe	Severe	Gilleron et al. (1997)
Methyl isobutyl ketone	108-10-1		100%					10.5	Severe	Severe	Gilleron et al. (1996)
Methyl isobutyl ketone	108-10-1		100%					17.75	Severe		Gilleron et al. (1997)
Methylpentynol	77-75-8	AP	100%	Liquid		soluble		20.1	Severe	Severe	Spielmann et al. (1996)
Methylpentynol	77-75-8	BD	100%	Liquid		soluble		12.9	Severe		Spielmann et al. (1996)

Substance Name	CASRN	Test Lab	Concentration Tested	Physical Form Tested	Purity (%)	Solubility[1]	pH	IS(B)-100[2]	IS(B)-100 Classification	Overall IS(B)-100 Classification	Reference
N-(2-methylphenyl)-Imidodi-carbonimidic diamide	93-69-6	AP	100%	Solid		40	11.5	4.7	Slight	Slight	Spielmann et al. (1996)
N-(2-methylphenyl)-Imidodi-carbonimidic diamide	93-69-6	MD	100%	Solid		40	11.5	n.p.			Spielmann et al. (1996)
2-Methyl-1-propanol	78-83-1	HK	100%	Liquid		15	3	20.4	Severe	Severe	Spielmann et al. (1996)
2-Methyl-1-propanol	78-83-1	MD	100%	Liquid		15	3	19.2	Severe		Spielmann et al. (1996)
Methyltriglycol	112-35-6	BD	100%	Liquid		readily soluble	7	12.5	Severe	Severe	Spielmann et al. (1996)
Methyltriglycol	112-35-6	HO	100%	Liquid		readily soluble	7	17	Severe		Spielmann et al. (1996)
Methyltriglycol	112-35-6	AP	100%	Liquid		readily soluble	7	20.4	Severe	Severe	Spielmann et al. (1996)
Methyltriglycol	112-35-6	HO	100%	Liquid		readily soluble	7	12.8	Severe		Spielmann et al. (1996)
MYRJ 45			100%					0	Nonirritant	Nonirritant	Gilleron et al. (1996)
Napt		HO	100%	Unknown		1000		10.3	Severe	Severe	Spielmann et al. (1996)
Napt		WA	100%	Unknown		1000		5.7	Moderate		Spielmann et al. (1996)
1-Naphthalene acetic acid	86-87-3		100%					7.46	Moderate	Moderate	Gilleron et al. (1997)
1-Naphthalene acetic acid, Na salt	61-31-4		100%					15.16	Severe	Severe	Gilleron et al. (1997)
Nitro-bis-octylamide		BG	100%	Unknown		insoluble		6.5	Moderate	Moderate	Spielmann et al. (1996)
Nitro-bis-octylamide		HK	100%	Unknown		insoluble		1.6	Slight		Spielmann et al. (1996)

Substance Name	CASRN	Test Lab	Concentration Tested	Physical Form Tested	Purity (%)	Solubility[1]	pH	IS(B)-100[2]	IS(B)-100 Classification	Overall IS(B)-100 Classification	Reference
1-Nitropropane	108-03-2		100%					2.8	Slight	Slight	Gilleron et al. (1996)
Octanol	111-87-5		100%					9.8	Severe	Severe	Gilleron et al. (1996)
Octanol	111-87-5		100%					16.7	Severe		Gilleron et al. (1997)
Oil/Water Emulsion-HZA			100%	Solution				1	Nonirritant	Slight	Gettings et al. (1994)
Oil/Water Emulsion-HZC			100%	Solution				3	Nonirritant	Slight	Gettings et al. (1994)
Oil/Water Emulsion-HZE			100%	Solution				3.67	Nonirritant	Slight	Gettings et al. (1994)
Oil/Water Emulsion-HZF			100%	Solution				3.67	Nonirritant	Slight	Gettings et al. (1994)
Oil/Water Emulsion-HZH			100%	Solution				23	Nonirritant	Severe	Gettings et al. (1994)
Oil/Water Emulsion-HZI			100%	Solution				0.333	Nonirritant	Nonirritant	Gettings et al. (1994)
Oil/Water Emulsion-HZJ			100%	Solution				3	Nonirritant	Slight	Gettings et al. (1994)
Oil/Water Emulsion-HZL			100%	Solution				10.3	Nonirritant	Severe	Gettings et al. (1994)
Oil/Water Emulsion-HZM			100%	Solution				14.3	Nonirritant	Severe	Gettings et al. (1994)
Oil/Water Emulsion-HZN			100%	Solution				3.67	Nonirritant	Slight	Gettings et al. (1994)
Oil/Water Emulsion-HZO			100%	Solution				0	Nonirritant	Nonirritant	Gettings et al. (1994)
Oil/Water Emulsion-HZR			100%	Solution				16.3	Category 1	Severe	Gettings et al. (1994)
Oil/Water Emulsion-HZS			100%	Solution				8.33	Nonirritant	Moderate	Gettings et al. (1994)

Substance Name	CASRN	Test Lab	Concentration Tested	Physical Form Tested	Purity (%)	Solubility[1]	pH	IS(B)-100[2]	IS(B)-100 Classification	Overall IS(B)-100 Classification	Reference
Oil/Water Emulsion-HZT			100%	Solution				1	Nonirritant	Slight	Gettings et al. (1994)
Oil/Water Emulsion-HZU			100%	Solution				1	Nonirritant	Slight	Gettings et al. (1994)
Oil/Water Emulsion-HZV			100%	Solution				0	Nonirritant	Nonirritant	Gettings et al. (1994)
Oil/Water Emulsion-HZW			100%	Solution				5	Nonirritant	Moderate	Gettings et al. (1994)
Oil/Water Emulsion-HZY			100%	Solution				9.67	Nonirritant	Severe	Gettings et al. (1994)
Olak		HK	100%	Unknown		soluble	8.3	19.5	Severe	Severe	Spielmann et al. (1996)
Olak		MD	100%	Unknown		soluble	8.3	17	Severe		Spielmann et al. (1996)
Ölesulf		BD	100%	Unknown		soluble	8	18.9	Severe	Severe	Spielmann et al. (1996)
Ölesulf		HK	100%	Unknown		soluble	8	19.6	Severe		Spielmann et al. (1996)
Parafluoraniline	371-40-4		100%					15.49	Severe	Severe	Gilleron et al. (1997)
2,4-Pentadione	123-54-6		100%					8.8	Moderate	Moderate	Gilleron et al. (1996)
Phenylephrine hydrochloride	61-76-7	AP	100%	Solid		1000	7	18.3	Severe	Severe	Spielmann et al. (1996)
Phenylephrine hydrochloride	61-76-7	HK	100%	Solid		1000	7	19.9	Severe		Spielmann et al. (1996)
1-Phenyl-3-pyrazolidine	92-43-3		100%					0.5	Nonirritant	Nonirritant	Gilleron et al. (1996)
Phenylthiourea	103-85-5	AP	100%	Solid		1	5.5	3.1	Slight	Slight	Spielmann et al. (1996)
Phenylthiourea	103-85-5	BD	100%	Solid		1	5.5	0	Nonirritant		Spielmann et al. (1996)

Substance Name	CASRN	Test Lab	Concentration Tested	Physical Form Tested	Purity (%)	Solubility[1]	pH	IS(B)-100[2]	IS(B)-100 Classification	Overall IS(B)-100 Classification	Reference
Phosphonat A		AP	100%	Unknown		3.6	2.1	3.5	Slight	Severe	Spielmann et al. (1996)
Phosphonat A		BG	100%	Unknown		3.6	2.1	10.1	Severe		Spielmann et al. (1996)
Acefyllin piperazinate	18833-13-1	HK	100%	Solid		625	5	15.3	Severe	Severe	Spielmann et al. (1996)
Acefyllin piperazinate	18833-13-1	WA	100%	Solid		625	5	14.6	Severe		Spielmann et al. (1996)
Acefyllin piperazinate	18833-13-1	BG	100%	Solid		625	5	9	Severe		Spielmann et al. (1996)
PO 2		AP	100%	Unknown		insoluble		0.3	Nonirritant	Nonirritant	Spielmann et al. (1996)
PO 2		WA	100%	Unknown		insoluble		0	Nonirritant		Spielmann et al. (1996)
Polyethylene glycol butyl ether	9004-77-7	AP	100%	Liquid		1000	6	19.3	Severe	Severe	Spielmann et al. (1996)
Polyethylene glycol butyl ether	9004-77-7	WA	100%	Liquid		1000	6	19.2	Severe		Spielmann et al. (1996)
Polyethylene glycol dimethyl ether	24991-55-7	HO	100%	Unknown		readily soluble	7	7.6	Moderate	Severe	Spielmann et al. (1996)
Polyethylene glycol dimethyl ether	24991-55-7	WA	100%	Unknown		readily soluble	7	19.8	Severe		Spielmann et al. (1996)
Polyethylene glycol	25322-68-3	MD	100%	Unknown		750		6.6	Moderate	Moderate	Spielmann et al. (1996)
Polyethylene glycol	25322-68-3	WA	100%	Unknown		750		7.7	Moderate		Spielmann et al. (1996)
Polyethylene glycol 400	25322-68-3		100%	Liquid				14.68	Severe		Gilleron et al. (1997)
Polyoxyethylene 23 lauryl ether	9002-92-0		100%					1.5	Slight	Slight	Gilleron et al. (1996)

Substance Name	CASRN	Test Lab	Concentration Tested	Physical Form Tested	Purity (%)	Solubility[1]	pH	IS(B)-100[2]	IS(B)-100 Classification	Overall IS(B)-100 Classification	Reference
Polyhexamethylene guanidine		BD	100%	Unknown		soluble	7.1	15.5	Severe	Severe	Spielmann et al. (1996)
Polyhexamethylene guanidine		BG	100%	Unknown		soluble	7.1	14.6	Severe		Spielmann et al. (1996)
Polysolvan	7397-62-8	AP	100%	Liquid		80	7	19.4	Severe	Severe	Spielmann et al. (1996)
Polysolvan	7397-62-8	HO	100%	Liquid		80	7	15.9	Severe		Spielmann et al. (1996)
Potassium cyanate	590-28-3	AP	100%	Solid		750	10	19.4	Severe	Severe	Spielmann et al. (1996)
Potassium cyanate	590-28-3	MD	100%	Solid		750	10	15.9	Severe		Spielmann et al. (1996)
Potassium cyanate	590-28-3		100%					14.27	Severe		Gilleron et al. (1997)
Potassium hexacyanoferrate II	14459-95-1	HK	100%	Solid		250	9.5	17.2	Severe	Severe	Spielmann et al. (1996)
Potassium hexacyanoferrate II	14459-95-1	HO	100%	Solid		250	9.5	6.3	Moderate		Spielmann et al. (1996)
Potassium hexacyanoferrate III	13756-66-2	BD	100%	Solid		310	8	5.7	Moderate	Moderate	Spielmann et al. (1996)
Potassium hexacyanoferrate III	13756-66-2	MD	100%	Solid		310	8	6.45	Moderate		Spielmann et al. (1996)
Promethazine HCl	58-33-3		100%					11.9	Severe	Severe	Gilleron et al. (1996)
Promethazine HCl	58-33-3		100%					6.27	Moderate		Gilleron et al. (1997)
Propyl-4-hydroxybenzoate	94-13-3		100%					1.9	Slight	Slight	Gilleron et al. (1996)
2-Pseudojonon		HK	100%	Unknown		0.1		7.3	Moderate	Moderate	Spielmann et al. (1996)
2-Pseudojonon		BG	100%	Unknown		0.1		4.1	Slight		Spielmann et al. (1996)

Substance Name	CASRN	Test Lab	Concentration Tested	Physical Form Tested	Purity (%)	Solubility[1]	pH	IS(B)-100[2]	IS(B)-100 Classification	Overall IS(B)-100 Classification	Reference
Pyridine	110-86-1		100%					15.8	Severe	Severe	Gilleron et al. (1996)
Pyridine	110-86-1		100%					17.79	Severe		Gilleron et al. (1997)
Quinacrine	69-05-6		100%					6.5	Moderate	Moderate	Gilleron et al. (1996)
Quinacrine	69-05-6		100%					7.29	Moderate		Gilleron et al. (1997)
RK Blau		HK	100%	Unknown		100	2.6	n.p.			Spielmann et al. (1996)
RK Blau		MD	100%	Unknown		100	2.6	n.p.			Spielmann et al. (1996)
Rubinrot Y		AP	100%	Unknown		172		5.3	Moderate	Moderate	Spielmann et al. (1996)
Rubinrot Y		HO	100%	Unknown		172		n.p.			Spielmann et al. (1996)
Sacyclo		HO	100%	Unknown		insoluble		4.4	Slight	Slight	Spielmann et al. (1996)
Sacyclo		MD	100%	Unknown		insoluble		3.3	Slight		Spielmann et al. (1996)
Sept		BD	100%	Unknown		soluble	3	15.9	Severe	Severe	Spielmann et al. (1996)
Sept		HK	100%	Unknown		soluble	3	19.8	Severe		Spielmann et al. (1996)
Sodium oxalate	62-76-0		100%					14.2	Severe	Severe	Gilleron et al. (1997)
Sodium perborate	10486-00-7		100%					13.19	Severe	Severe	Gilleron et al. (1997)
Tetraaminopyrimidine sulfate	5392-28-9		100%					0.5	Nonirritant	Slight	Gilleron et al. (1996)
Tetraaminopyrimidine sulfate	5392-28-9		100%					4.33	Slight		Gilleron et al. (1997)

Substance Name	CASRN	Test Lab	Concentration Tested	Physical Form Tested	Purity (%)	Solubility[1]	pH	IS(B)-100[2]	IS(B)-100 Classification	Overall IS(B)-100 Classification	Reference
Thiourea	62-56-6		100%					13.7	Severe	Severe	Gilleron et al. (1996)
Thiourea	62-56-6		100%					17.89	Severe		Gilleron et al. (1997)
Toluene	108-88-3		100%					16.09	Severe	Severe	Gilleron et al. (1997)
1,2,3-Trichloropropane	96-18-4		100%					7.9	Moderate	Moderate	Gilleron et al. (1996)
1,2,4-Trichloropropane	95-63-6		100%					4.5	Slight	Slight	Gilleron et al. (1996)
Triethanolamine	102-71-6		100%					9.6	Severe	Severe	Gilleron et al. (1996)
Trimethoxypropylsilane	1067-25-0	BD	100%	Liquid		poorly soluble		4.5	Slight	Severe	Spielmann et al. (1996)
Trimethoxypropylsilane	1067-25-0	AP	100%	Liquid		poorly soluble		13.7	Severe		Spielmann et al. (1996)
Trimethoxyoctylsilane	3069-40-7	HO	100%	Liquid		insoluble		8.4	Moderate	Severe	Spielmann et al. (1996)
Trimethoxyoctylsilane	3069-40-7	BG	100%	Liquid		insoluble		10	Severe		Spielmann et al. (1996)
Silan 165	29055-11-6	HO	100%	Unknown		insoluble		4.1	Slight	Moderate	Spielmann et al. (1996)
Silan 165	29055-11-6	WA	100%	Unknown		insoluble		7.2	Moderate		Spielmann et al. (1996)
Silan 167	41453-78-5	WA	100%	Unknown		soluble		4.7	Slight	Slight	Spielmann et al. (1996)
Silan 167	41453-78-5	HO	100%	Unknown		soluble		2.3	Slight		Spielmann et al. (1996)
Silan 253	18784-74-2	BD	100%	Unknown		insoluble	<7	9.9	Severe	Severe	Spielmann et al. (1996)
Silan 253	18784-74-2	MD	100%	Unknown		insoluble	<7	14.7	Severe		Spielmann et al. (1996)

Substance Name	CASRN	Test Lab	Concentration Tested	Physical Form Tested	Purity (%)	Solubility[1]	pH	IS(B)-100[2]	IS(B)-100 Classification	Overall IS(B)-100 Classification	Reference
Sodium bisulfite	7631-90-5	AP	100%	Solid		readily soluble	4.5	20	Severe	Severe	Spielmann et al. (1996)
Sodium bisulfite	7631-90-5	MD	100%	Solid		readily soluble	4.5	16.8	Severe		Spielmann et al. (1996)
Sodium sulfite	7757-83-7	AP	100%	Solid		250	10	16.1	Severe	Severe	Spielmann et al. (1996)
Sodium sulfite	7757-83-7	BG	100%	Solid		250	10	12.3	Severe		Spielmann et al. (1996)
Sodium cyanate	917-61-3	MD	100%	Solid		110	10.4	8.2	Moderate	Severe	Spielmann et al. (1996)
Sodium cyanate	917-61-3	WA	100%	Solid		110	10.4	10.7	Severe		Spielmann et al. (1996)
Sodium disilicate	13870-28-5	BG	100%	Solid		3.5	11.4	18.2	Severe	Severe	Spielmann et al. (1996)
Sodium disilicate	13870-28-5	HK	100%	Solid		3.5	11.4	16.6	Severe		Spielmann et al. (1996)
Sodium hydrogen sulfate	7681-38-1	HK	100%	Solid		1080	1.1	19.2	Severe	Severe	Spielmann et al. (1996)
Sodium hydrogen sulfate	7681-38-1	WA	100%	Solid		1080	1.1	18.1	Severe		Spielmann et al. (1996)
Sodium lauryl ether sulfate	3088-31-1	BG	100%	Unknown		soluble	8	17.9	Severe	Severe	Spielmann et al. (1996)
Sodium lauryl ether sulfate	3088-31-1	MD	100%	Unknown		soluble	8	19	Severe		Spielmann et al. (1996)
Sodium monochloroacetate	3926-62-3	HO	100%	Solid		440	4.5	16.1	Severe	Severe	Spielmann et al. (1996)
Sodium monochloroacetate	3926-62-3	BD	100%	Solid		440	4.5	10.8	Severe		Spielmann et al. (1996)

Substance Name	CASRN	Test Lab	Concentration Tested	Physical Form Tested	Purity (%)	Solubility[1]	pH	IS(B)-100[2]	IS(B)-100 Classification	Overall IS(B)-100 Classification	Reference
Sodiumpyrosulfite	7681-57-4	AP	100%	Solid		650	4.6	17.7	Severe	Severe	Spielmann et al. (1996)
Sodiumpyrosulfite	7681-57-4	BD	100%	Solid		650	4.6	11.6	Severe		Spielmann et al. (1996)
Sodiumpyrosulfite	7681-57-4	bg	100%	Solid		650	4.6	14.5	Severe		Spielmann et al. (1996)
4-((2-sulfatoethyl)sulfonyl)-aniline	2494-89-5	AP	100%	Unknown		soluble	7	10.4	Severe	Severe	Spielmann et al. (1996)
4-((2-sulfatoethyl)sulfonyl)-aniline	2494-89-5	HK	100%	Unknown		soluble	7	n.p.	Severe		Spielmann et al. (1996)
TA 01946 Alkylsilan		AP	100%	Unknown		0.014		16.2	Severe	Severe	Spielmann et al. (1996)
TA 01946 Alkylsilan		HK	100%	Unknown		0.014		10	Severe		Spielmann et al. (1996)
Theophylline sodium acetate	8002-89-9	AP	100%	Unknown		50	11	6.9	Moderate	Moderate	Spielmann et al. (1996)
Theophylline sodium acetate	8002-89-9	HO	100%	Unknown		50	11	n.p.	Severe		Spielmann et al. (1996)
Tocla		BD	100%	Unknown		40	6	13.5	Severe	Severe	Spielmann et al. (1996)
Tocla		HK	100%	Unknown		40	6	20.4	Severe		Spielmann et al. (1996)
Triisooctylamine	25549-16-0	BG	100%	Solid		0.5	7	14.1	Severe	Severe	Spielmann et al. (1996)
Triisooctylamine	25549-16-0	MD	100%	Solid		0.5	7	4	Slight		Spielmann et al. (1996)
2,2,3-Trimethyl-3-Cyclo-pentene-1-acetaldehyde	4501-58-0	BG	100%	Solid		< 2.5	2.3	9.7	Severe	Severe	Spielmann et al. (1996)
2,2,3-Trimethyl-3-Cyclo-pentene-1-acetaldehyde	4501-58-0	AP	100%	Solid		< 2.5	2.3	14.7	Severe		Spielmann et al. (1996)

Substance Name	CASRN	Test Lab	Concentration Tested	Physical Form Tested	Purity (%)	Solubility[1]	pH	IS(B)-100[2]	IS(B)-100 Classification	Overall IS(B)-100 Classification	Reference
Trioxane	110-88-3	HK	100%	Solid		172		18	Severe	Severe	Spielmann et al. (1996)
Trioxane	110-88-3	WA	100%	Solid		172		17.8	Severe		Spielmann et al. (1996)
Triton X-155	9010-44-0		100%					3.9	Slight	Slight	Gilleron et al. (1996)
Tween 20	9005-64-5		100%					14.47	Severe	Severe	Gilleron et al. (1997)
Tween 20	9005-64-5		100%					3.22	Slight		Vinardell and Macián (1994)
Wessalith Slurry		BG	100%	Unknown		readily soluble	11	4.1	Slight	Severe	Spielmann et al. (1996)
Wessalith Slurry		WA	100%	Unknown		readily soluble	11	15.7	Severe		Spielmann et al. (1996)
Xanthinol nicotinate	437-74-1	WA	100%	Solid		250	6	9	Severe	Severe	Spielmann et al. (1996)
Xanthinol nicotinate	437-74-1	HK	100%	Solid		250	6	17.4	Severe		Spielmann et al. (1996)

Abbreviations: CASRN = Chemical Abstracts Service Registry Number.

[1] Solubility = obtained from literature references, where available, expressed as g/mL

[2] IS(B)-100 represents irritation scores that were calculated using a method similar to the one described in Kalweit et al. (1987) where the *in vitro* scores was obtained using a 100% concentration and where the *in vivo* results were obtained at 100% concentration.

Appendix C9

Data Sorted by Substance for Q-Score Analysis Method

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Substance Name	CASRN	Lab Number	*In Vitro* Concentration Tested	*In Vitro* Physical Form Tested	Purity (%)	Solubility[1]	pH	Q-Score[2]	Q-Score Classification	Overall Q-Score Classification	Reference
Acetone	67-64-1	1	100%	Liquid	>99	water soluble		18.36	Severe	Severe	Balls et al. (1995)
Acetone	67-64-1	2	100%	Liquid	>99	water soluble		13.53	Severe		Balls et al. (1995)
Acetone	67-64-1	3	100%	Liquid	>99	water soluble		0.80	Nonirritant		Balls et al. (1995)
Acetone	67-64-1	4	100%	Liquid	>99	water soluble		10.31	Severe		Balls et al. (1995)
Ammonium nitrate	6484-52-2	1	100%	Solid	>99.9	water soluble		1.80	Moderate	Moderate	Balls et al. (1995)
Ammonium nitrate	6484-52-2	3	100%	Solid	>99.9	water soluble		1.30	Nonirritant		Balls et al. (1995)
L-Aspartic acid	70-47-3	1	100%	Solid	95	water soluble		0.00	Nonirritant	Nonirritant	Balls et al. (1995)
Benzalkonium chloride	8001-54-5	1	1%	Solution	98	surfactant		3.41	Severe	Severe	Balls et al. (1995)
Benzalkonium chloride	8001-54-5	2	1%	Solution	98	surfactant		5.00	Severe		Balls et al. (1995)
Benzalkonium chloride	8001-54-5	3	1%	Solution	98	surfactant		3.90	Severe		Balls et al. (1995)
Benzalkonium chloride	8001-54-5	4	1%	Solution	98	surfactant		4.39	Severe		Balls et al. (1995)
Benzalkonium chloride	8001-54-5	1	5%	Solution	98	surfactant		6.93	Severe	Severe	Balls et al. (1995)
Benzalkonium chloride	8001-54-5	2	5%	Solution	98	surfactant		4.43	Severe		Balls et al. (1995)
Benzalkonium chloride	8001-54-5	3	5%	Solution	98	surfactant		1.20	Nonirritant		Balls et al. (1995)
Benzalkonium chloride	8001-54-5	4	5%	Solution	98	surfactant		6.49	Severe		Balls et al. (1995)
Benzalkonium chloride	8001-54-5	1	10%	Solution	98	surfactant		6.09	Severe	Severe	Balls et al. (1995)
Benzalkonium chloride	8001-54-5	2	10%	Solution	98	surfactant		7.03	Severe		Balls et al. (1995)
Benzalkonium chloride	8001-54-5	3	10%	Solution	98	surfactant		3.10	Severe		Balls et al. (1995)
Benzalkonium chloride	8001-54-5	4	10%	Solution	98	surfactant		6.14	Severe		Balls et al. (1995)
Butyl acetate	123-86-4	1	100%	Liquid	99	water insoluble		1.55	Moderate	Moderate	Balls et al. (1995)
Butyl acetate	123-86-4	2	100%	Liquid	99	water insoluble		1.23	Nonirritant		Balls et al. (1995)
Butyl acetate	123-86-4	3	100%	Liquid	99	water insoluble		1.80	Moderate		Balls et al. (1995)
Butyl acetate	123-86-4	4	100%	Liquid	99	water insoluble		1.93	Moderate		Balls et al. (1995)
Gamma-butyrolactone	96-48-0	1	100%	Liquid	>99	water soluble		22.04	Severe	Severe	Balls et al. (1995)
Gamma-butyrolactone	96-48-0	2	100%	Liquid	>99	water soluble		6.64	Severe		Balls et al. (1995)
Gamma-butyrolactone	96-48-0	3	100%	Liquid	>99	water soluble		1.97	Moderate		Balls et al. (1995)
Gamma-butyrolactone	96-48-0	4	100%	Liquid	>99	water soluble		4.02	Severe		Balls et al. (1995)
Cetylpyridinium bromide	140-72-7	1	0.10%	Solution	98	surfactant		2.43	Severe	Nonirritant	Balls et al. (1995)
Cetylpyridinium bromide	140-72-7	2	0.10%	Solution	98	surfactant		0.00	Nonirritant		Balls et al. (1995)
Cetylpyridinium bromide	140-72-7	3	0.10%	Solution	98	surfactant		1.00	Nonirritant		Balls et al. (1995)
Cetylpyridinium bromide	140-72-7	4	0.10%	Solution	98	surfactant		0.00	Nonirritant		Balls et al. (1995)
Cetylpyridinium bromide	140-72-7	1	6%	Solution	98	surfactant		2.34	Severe	Severe	Balls et al. (1995)
Cetylpyridinium bromide	140-72-7	2	6%	Solution	98	surfactant		2.42	Severe		Balls et al. (1995)
Cetylpyridinium bromide	140-72-7	3	6%	Solution	98	surfactant		1.30	Nonirritant		Balls et al. (1995)
Cetylpyridinium bromide	140-72-7	4	6%	Solution	98	surfactant		3.11	Severe		Balls et al. (1995)

Substance Name	CASRN	Lab Number	*In Vitro* Concentration Tested	*In Vitro* Physical Form Tested	Purity (%)	Solubility[1]	pH	Q-Score[2]	Q-Score Classification	Overall Q-Score Classification	Reference
Cetylpyridinium bromide	140-72-7	1	10%	Solution	98	surfactant		2.71	Severe	Severe	Balls et al. (1995)
Cetylpyridinium bromide	140-72-7	2	10%	Solution	98	surfactant		2.73	Severe		Balls et al. (1995)
Cetylpyridinium bromide	140-72-7	3	10%	Solution	98	surfactant		1.80	Moderate		Balls et al. (1995)
Cetylpyridinium bromide	140-72-7	4	10%	Solution	98	surfactant		4.67	Severe		Balls et al. (1995)
Cyclohexanol	108-93-0	1	100%	Liquid	97	water soluble		3.28	Severe	Severe	Balls et al. (1995)
Cyclohexanol	108-93-0	2	100%	Liquid	97	water soluble		4.48	Severe		Balls et al. (1995)
Cyclohexanol	108-93-0	3	100%	Liquid	97	water soluble		5.20	Severe		Balls et al. (1995)
Cyclohexanol	108-93-0	4	100%	Liquid	97	water soluble		6.69	Severe		Balls et al. (1995)
2,6-Dichlorobenzoyl chloride	4659-45-4	1	100%	Liquid	99	water insoluble		10.14	Severe	Severe	Balls et al. (1995)
2,6-Dichlorobenzoyl chloride	4659-45-4	2	100%	Liquid	99	water insoluble		8.81	Severe		Balls et al. (1995)
2,6-Dichlorobenzoyl chloride	4659-45-4	3	100%	Liquid	99	water insoluble		1.90	Moderate		Balls et al. (1995)
2,6-Dichlorobenzoyl chloride	4659-45-4	4	100%	Liquid	99	water insoluble		2.53	Severe		Balls et al. (1995)
2,2-Dimethylbutanoic acid	595-37-9	1	100%	Liquid	>99	water insoluble		14.05	Severe	Severe	Balls et al. (1995)
2,2-Dimethylbutanoic acid	595-37-9	2	100%	Liquid	>99	water insoluble		10.64	Severe		Balls et al. (1995)
2,2-Dimethylbutanoic acid	595-37-9	3	100%	Liquid	>99	water insoluble		11.70	Severe		Balls et al. (1995)
2,2-Dimethylbutanoic acid	595-37-9	4	100%	Liquid	>99	water insoluble		14.73	Severe		Balls et al. (1995)
2,5-Dimethylhexanediol	110-03-2	1	100%	Solid	99.5	water insoluble		2.07	Severe	Severe	Balls et al. (1995)
2,5-Dimethylhexanediol	110-03-2	3	100%	Solid	99.5	water insoluble		0.80	Nonirritant		Balls et al. (1995)

Substance Name	CASRN	Lab Number	*In Vitro* Concentration Tested	*In Vitro* Physical Form Tested	Purity (%)	Solubility[1]	pH	Q-Score[2]	Q-Score Classification	Overall Q-Score Classification	Reference
Ethanol	64-17-5	1	100%	Liquid		water soluble		6.45	Severe	Severe	Balls et al. (1995)
Ethanol	64-17-5	2	100%	Liquid		water soluble		10.63	Severe		Balls et al. (1995)
Ethanol	64-17-5	3	100%	Liquid		water soluble		1.47	Nonirritant		Balls et al. (1995)
Ethanol	64-17-5	4	100%	Liquid		water soluble		5.95	Severe		Balls et al. (1995)
Ethyl acetate	141-78-6	1	100%	Liquid	99	water soluble		3.94	Severe	Severe	Balls et al. (1995)
Ethyl acetate	141-78-6	2	100%	Liquid	99	water soluble		1.87	Moderate		Balls et al. (1995)
Ethyl acetate	141-78-6	3	100%	Liquid	99	water soluble		0.90	Nonirritant		Balls et al. (1995)
Ethyl acetate	141-78-6	4	100%	Liquid	99	water soluble		3.37	Severe		Balls et al. (1995)
2-Ethyl-1-hexanol	104-76-7	1	100%	Liquid	99	water soluble		1.24	Nonirritant	Nonirritant	Balls et al. (1995)
2-Ethyl-1-hexanol	104-76-7	2	100%	Liquid	99	water soluble		0.61	Nonirritant		Balls et al. (1995)
2-Ethyl-1-hexanol	104-76-7	3	100%	Liquid	99	water soluble		1.00	Nonirritant		Balls et al. (1995)
2-Ethyl-1-hexanol	104-76-7	4	100%	Liquid	99	water soluble		3.12	Severe		Balls et al. (1995)
Ethyl-2-methylacetoacetate	609-14-3	1	100%	Liquid	ca. 97	water soluble		2.40	Severe	Severe	Balls et al. (1995)
Ethyl-2-methylacetoacetate	609-14-3	2	100%	Liquid	ca. 97	water soluble		2.51	Severe		Balls et al. (1995)
Ethyl-2-methylacetoacetate	609-14-3	3	100%	Liquid	ca. 97	water soluble		1.10	Nonirritant		Balls et al. (1995)
Ethyl-2-methylacetoacetate	609-14-3	4	100%	Liquid	ca. 97	water soluble		2.35	Severe		Balls et al. (1995)
Ethyl trimethyl acetate	3938-95-2	1	100%	Liquid	99	water insoluble		0.10	Nonirritant	Nonirritant	Balls et al. (1995)
Ethyl trimethyl acetate	3938-95-2	2	100%	Liquid	99	water insoluble		0.19	Nonirritant		Balls et al. (1995)
Ethyl trimethyl acetate	3938-95-2	3	100%	Liquid	99	water insoluble		0.30	Nonirritant		Balls et al. (1995)
Ethyl trimethyl acetate	3938-95-2	4	100%	Liquid	99	water insoluble		1.01	Nonirritant		Balls et al. (1995)

Substance Name	CASRN	Lab Number	*In Vitro* Concentration Tested	*In Vitro* Physical Form Tested	Purity (%)	Solubility[1]	pH	Q-Score[2]	Q-Score Classification	Overall Q-Score Classification	Reference
Glycerol	56-81-5	1	100%	Liquid	>99.5	water soluble		0.08	Nonirritant	Nonirritant	Balls et al. (1995)
Glycerol	56-81-5	2	100%	Liquid	>99.5	water soluble		1.24	Nonirritant		Balls et al. (1995)
Glycerol	56-81-5	3	100%	Liquid	>99.5	water soluble		0.60	Nonirritant		Balls et al. (1995)
Glycerol	56-81-5	4	100%	Liquid	>99.5	water soluble		1.22	Nonirritant		Balls et al. (1995)
Hexanol	111-27-3	1	100%	Liquid	98	water insoluble		5.01	Severe	Severe	Balls et al. (1995)
Hexanol	111-27-3	2	100%	Liquid	98	water insoluble		3.98	Severe		Balls et al. (1995)
Hexanol	111-27-3	3	100%	Liquid	98	water insoluble		1.80	Moderate		Balls et al. (1995)
Hexanol	111-27-3	4	100%	Liquid	98	water insoluble		4.71	Severe		Balls et al. (1995)
Imidazole	288-32-4	1	100%	Solid	99	water soluble		11.19	Severe	Severe	Balls et al. (1995)
Imidazole	288-32-4	3	100%	Solid	99	water soluble		3.50	Severe		Balls et al. (1995)
Isobutanol	78-83-1	1	100%	Liquid	99.9	water insoluble		4.59	Severe	Severe	Balls et al. (1995)
Isobutanol	78-83-1	2	100%	Liquid	99.9	water insoluble		3.58	Severe		Balls et al. (1995)
Isobutanol	78-83-1	3	100%	Liquid	99.9	water insoluble		1.20	Nonirritant		Balls et al. (1995)
Isobutanol	78-83-1	4	100%	Liquid	99.9	water insoluble		5.89	Severe		Balls et al. (1995)
Isopropanol	67-63-0	1	100%	Liquid	99.9	water soluble		11.90	Severe	Severe	Balls et al. (1995)
Isopropanol	67-63-0	2	100%	Liquid	99.9	water soluble		5.79	Severe		Balls et al. (1995)
Isopropanol	67-63-0	3	100%	Liquid	99.9	water soluble		1.80	Moderate		Balls et al. (1995)
Isopropanol	67-63-0	4	100%	Liquid	99.9	water soluble		4.36	Severe		Balls et al. (1995)
Maneb	12427-38-2	1	100%	Solid	90	water soluble		0.00	Nonirritant	Nonirritant	Balls et al. (1995)

Substance Name	CASRN	Lab Number	*In Vitro* Concentration Tested	*In Vitro* Physical Form Tested	Purity (%)	Solubility[1]	pH	Q-Score[2]	Q-Score Classification	Overall Q-Score Classification	Reference
Methyl acetate	79-20-9	1	100%	Liquid	98	water soluble		1.88	Moderate	Severe	Balls et al. (1995)
Methyl acetate	79-20-9	2	100%	Liquid	98	water soluble		5.39	Severe		Balls et al. (1995)
Methyl acetate	79-20-9	3	100%	Liquid	98	water soluble		1.70	Moderate		Balls et al. (1995)
Methyl acetate	79-20-9	4	100%	Liquid	98	water soluble		3.15	Severe		Balls et al. (1995)
Methyl cyanoacetate	105-34-0	1	100%	Liquid	99	water soluble		1.51	Moderate	Moderate	Balls et al. (1995)
Methyl cyanoacetate	105-34-0	2	100%	Liquid	99	water soluble		1.21	Nonirritant		Balls et al. (1995)
Methyl cyanoacetate	105-34-0	3	100%	Liquid	99	water soluble		1.00	Nonirritant		Balls et al. (1995)
Methyl cyanoacetate	105-34-0	4	100%	Liquid	99	water soluble		1.78	Moderate		Balls et al. (1995)
Methylcyclopentane	96-37-7	1	100%	Liquid	>99	water insoluble		0.18	Nonirritant	Nonirritant	Balls et al. (1995)
Methylcyclopentane	96-37-7	2	100%	Liquid	>99	water insoluble		1.22	Nonirritant		Balls et al. (1995)
Methylcyclopentane	96-37-7	3	100%	Liquid	>99	water insoluble		0.20	Nonirritant		Balls et al. (1995)
Methylcyclopentane	96-37-7	4	100%	Liquid	>99	water insoluble		8.09	Severe		Balls et al. (1995)
Methyl ethyl ketone	78-93-3	1	100%	Liquid	99	water soluble		5.83	Severe	Severe	Balls et al. (1995)
Methyl ethyl ketone	78-93-3	2	100%	Liquid	99	water soluble		3.89	Severe		Balls et al. (1995)
Methyl ethyl ketone	78-93-3	3	100%	Liquid	99	water soluble		2.50	Severe		Balls et al. (1995)
Methyl ethyl ketone	78-93-3	4	100%	Liquid	99	water soluble		6.17	Severe		Balls et al. (1995)

Substance Name	CASRN	Lab Number	*In Vitro* Concentration Tested	*In Vitro* Physical Form Tested	Purity (%)	Solubility[1]	pH	Q-Score[2]	Q-Score Classification	Overall Q-Score Classification	Reference
Methyl isobutyl ketone	108-10-1	1	100%	Liquid	98	water insoluble		2.29	Severe	Moderate	Balls et al. (1995)
Methyl isobutyl ketone	108-10-1	2	100%	Liquid	98	water insoluble		1.04	Nonirritant		Balls et al. (1995)
Methyl isobutyl ketone	108-10-1	3	100%	Liquid	98	water insoluble		1.50	Moderate		Balls et al. (1995)
Methyl isobutyl ketone	108-10-1	4	100%	Liquid	98	water insoluble		1.86	Moderate		Balls et al. (1995)
1-Naphthalene acetic acid, Na salt	61-31-4	1	100%	Solid	95	water soluble		3.84	Severe	Severe	Balls et al. (1995)
1-Naphthalene acetic acid, Na salt	61-31-4	3	100%	Solid	95	water soluble		4.90	Severe		Balls et al. (1995)
Octanol	111-87-5	1	100%	Liquid	>99	water insoluble		2.10	Severe	Moderate	Balls et al. (1995)
Octanol	111-87-5	2	100%	Liquid	>99	water insoluble		1.00	Nonirritant		Balls et al. (1995)
Octanol	111-87-5	3	100%	Liquid	>99	water insoluble		1.80	Moderate		Balls et al. (1995)
Octanol	111-87-5	4	100%	Liquid	>99	water insoluble		1.78	Moderate		Balls et al. (1995)
Parafluoraniline	371-40-4	1	100%	Liquid	99	water insoluble		5.25	Severe	Severe	Balls et al. (1995)
Parafluoraniline	371-40-4	2	100%	Liquid	99	water insoluble		4.46	Severe		Balls et al. (1995)
Parafluoraniline	371-40-4	3	100%	Liquid	99	water insoluble		1.90	Moderate		Balls et al. (1995)
Parafluoraniline	371-40-4	4	100%	Liquid	99	water insoluble		2.57	Severe		Balls et al. (1995)
Polyethylene glycol 400	25322-68-3	1	100%	Liquid		surfactant		1.59	Moderate	Nonirritant	Balls et al. (1995)
Polyethylene glycol 400	25322-68-3	2	100%	Liquid		surfactant		0.72	Nonirritant		Balls et al. (1995)
Polyethylene glycol 400	25322-68-3	3	100%	Liquid		surfactant		0.60	Nonirritant		Balls et al. (1995)
Polyethylene glycol 400	25322-68-3	4	100%	Liquid		surfactant		1.22	Nonirritant		Balls et al. (1995)
Potassium cyanate	590-28-3	1	100%	Solid	97	water soluble		2.17	Severe	Severe	Balls et al. (1995)
Potassium cyanate	590-28-3	3	100%	Solid	97	water soluble		2.50	Severe		Balls et al. (1995)
Potassium cyanate	590-28-3	4	100%	Solid	97	water soluble		6.07	Severe		Balls et al. (1995)
Promethazine HCl	58-33-3	1	100%	Solid	100	water soluble		3.20	Severe	Severe	Balls et al. (1995)
Promethazine HCl	58-33-3	3	100%	Solid	100	water soluble		3.00	Severe		Balls et al. (1995)

Substance Name	CASRN	Lab Number	*In Vitro* Concentration Tested	*In Vitro* Physical Form Tested	Purity (%)	Solubility[1]	pH	Q-Score[2]	Q-Score Classification	Overall Q-Score Classification	Reference
Pyridine	110-86-1	1	100%	Liquid	>99.9	water soluble		3.84	Severe	Severe	Balls et al. (1995)
Pyridine	110-86-1	2	100%	Liquid	>99.9	water soluble		7.76	Severe		Balls et al. (1995)
Pyridine	110-86-1	3	100%	Liquid	>99.9	water soluble		12.90	Severe		Balls et al. (1995)
Pyridine	110-86-1	4	100%	Liquid	>99.9	water soluble		10.44	Severe		Balls et al. (1995)
Sodium hydroxide	1310-73-2	1	1%	Solution		water soluble		6.34	Severe	Severe	Balls et al. (1995)
Sodium hydroxide	1310-73-2	2	1%	Solution		water soluble		6.17	Severe		Balls et al. (1995)
Sodium hydroxide	1310-73-2	3	1%	Solution		water soluble		4.80	Severe		Balls et al. (1995)
Sodium hydroxide	1310-73-2	4	1%	Solution		water soluble		4.36	Severe		Balls et al. (1995)
Sodium hydroxide	1310-73-2	1	10%	Solution		water soluble		13.13	Severe	Severe	Balls et al. (1995)
Sodium hydroxide	1310-73-2	2	10%	Solution		water soluble		7.82	Severe		Balls et al. (1995)
Sodium hydroxide	1310-73-2	3	10%	Solution		water soluble		23.00	Severe		Balls et al. (1995)
Sodium hydroxide	1310-73-2	4	10%	Solution		water soluble		9.82	Severe		Balls et al. (1995)
Sodium lauryl sulfate	151-21-3	1	3%	Solution	98	surfactant		2.68	Severe	Severe	Balls et al. (1995)
Sodium lauryl sulfate	151-21-3	2	3%	Solution	98	surfactant		1.62	Moderate		Balls et al. (1995)
Sodium lauryl sulfate	151-21-3	3	3%	Solution	98	surfactant		1.70	Moderate		Balls et al. (1995)
Sodium lauryl sulfate	151-21-3	4	3%	Solution	98	surfactant		2.46	Severe		Balls et al. (1995)
Sodium lauryl sulfate	151-21-3	1	15%	Solution	98	surfactant		2.86	Severe	Severe	Balls et al. (1995)
Sodium lauryl sulfate	151-21-3	2	15%	Solution	98	surfactant		2.34	Severe		Balls et al. (1995)
Sodium lauryl sulfate	151-21-3	3	15%	Solution	98	surfactant		1.80	Moderate		Balls et al. (1995)
Sodium lauryl sulfate	151-21-3	4	15%	Solution	98	surfactant		4.37	Severe		Balls et al. (1995)
Thiourea	62-56-6	1	100%	Solid	>99	water soluble		1.31	Nonirritant	Nonirritant	Balls et al. (1995)
Thiourea	62-56-6	3	100%	Solid	>99	water soluble		0.50	Nonirritant		Balls et al. (1995)
Toluene	108-88-3	1	100%	Liquid	99	water insoluble		3.18	Severe	Severe	Balls et al. (1995)
Toluene	108-88-3	2	100%	Liquid	99	water insoluble		5.84	Severe		Balls et al. (1995)
Toluene	108-88-3	3	100%	Liquid	99	water insoluble		2.90	Severe		Balls et al. (1995)
Toluene	108-88-3	4	100%	Liquid	99	water insoluble		2.98	Severe		Balls et al. (1995)
Trichloroacetic acid	76-03-9	1	3%	Solution		water soluble		18.76	Severe	Severe	Balls et al. (1995)
Trichloroacetic acid	76-03-9	2	3%	Solution		water soluble		9.15	Severe		Balls et al. (1995)
Trichloroacetic acid	76-03-9	3	3%	Solution		water soluble		9.90	Severe		Balls et al. (1995)
Trichloroacetic acid	76-03-9	4	3%	Solution		water soluble		5.33	Severe		Balls et al. (1995)
Trichloroacetic acid	76-03-9	1	30%	Solution		water soluble		14.39	Severe	Severe	Balls et al. (1995)
Trichloroacetic acid	76-03-9	2	30%	Solution		water soluble		9.96	Severe		Balls et al. (1995)
Trichloroacetic acid	76-03-9	3	30%	Solution		water soluble		13.10	Severe		Balls et al. (1995)
Trichloroacetic acid	76-03-9	4	30%	Solution		water soluble		11.81	Severe		Balls et al. (1995)
Triton X-100	9002-93-1	1	5%	Solution	98	surfactant		2.66	Severe	Severe	Balls et al. (1995)
Triton X-100	9002-93-1	2	5%	Solution	98	surfactant		2.72	Severe		Balls et al. (1995)
Triton X-100	9002-93-1	3	5%	Solution	98	surfactant		1.40	Nonirritant		Balls et al. (1995)
Triton X-100	9002-93-1	4	5%	Solution	98	surfactant		2.20	Severe		Balls et al. (1995)
Triton X-100	9002-93-1	1	10%	Solution	98	surfactant		3.45	Severe	Severe	Balls et al. (1995)
Triton X-100	9002-93-1	2	10%	Solution	98	surfactant		1.71	Moderate		Balls et al. (1995)
Triton X-100	9002-93-1	3	10%	Solution	98	surfactant		1.70	Moderate		Balls et al. (1995)
Triton X-100	9002-93-1	4	10%	Solution	98	surfactant		2.40	Severe		Balls et al. (1995)
Tween 20	9005-64-5	1	100%	Liquid	98	surfactant		0.39	Nonirritant	Nonirritant	Balls et al. (1995)
Tween 20	9005-64-5	2	100%	Liquid	98	surfactant		0.38	Nonirritant		Balls et al. (1995)
Tween 20	9005-64-5	3	100%	Liquid	98	surfactant		0.60	Nonirritant		Balls et al. (1995)
Tween 20	9005-64-5	4	100%	Liquid	98	surfactant		0.95	Nonirritant		Balls et al. (1995)

Abbreviation: CASRN = Chemical Abstract Service Registry Number, HCl = Hydrochloric acid.

[1] Solubility obtained from literature references, where availble, expressed as g/mL

[2] Q-Score represents irritation scores that were calcualted using the method described in Balls et al. (1995)

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Appendix C10

Data Sorted by Substance for S-Score Analysis Method

Substance Name	CASRN	*In Vitro* Concentration Tested	*In Vitro* Physical Form Tested	Purity (%)	Solubility[1]	pH	S-Score[2]	S-Score Classification	Overall S-Score Classification	Reference
Ammonium nitrate	6484-52-2	100%	Solid	>99.9	water soluble		18.00	Severe	Severe	Balls et al. (1995)
Ammonium nitrate	6484-52-2	100%	Solid	>99.9	water soluble		12.00	Moderate		Balls et al. (1995)
L-Aspartic acid	70-47-3	100%	Solid	100	water soluble		1.00	Nonirritant	Nonirritant	Balls et al. (1995)
L-Aspartic acid	70-47-3	100%	Solid	100	water soluble		2.00	Nonirritant		Balls et al. (1995)
L-Aspartic acid	70-47-3	100%	Solid	100	water soluble		6.00	Moderate		Balls et al. (1995)
Benzoyl-L-tartaric acid	2743-38-6	100%	Solid	98	water insoluble		0.00	Nonirritant	Nonirritant	Balls et al. (1995)
Benzoyl-L-tartaric acid	2743-38-6	100%	Solid	98	water insoluble		4.00	Nonirritant		Balls et al. (1995)
Captan 90 concentrate	133-06-2	100%	Solid	90	water soluble		0.00	Nonirritant	Nonirritant	Balls et al. (1995)
Captan 90 concentrate	133-06-2	100%	Solid	90	water soluble		0.00	Nonirritant		Balls et al. (1995)
Captan 90 concentrate	133-06-2	100%	Solid	90	water soluble		6.00	Moderate		Balls et al. (1995)
4-Carboxybenzaldehyde	619-66-9	100%	Solid	95	water insoluble		0.00	Nonirritant	Moderate	Balls et al. (1995)
4-Carboxybenzaldehyde	619-66-9	100%	Solid	95	water insoluble		6.00	Moderate		Balls et al. (1995)
4-Carboxybenzaldehyde	619-66-9	100%	Solid	95	water insoluble		6.00	Moderate		Balls et al. (1995)
4-Carboxybenzaldehyde	619-66-9	100%	Solid	95	water insoluble		4.00	Nonirritant		Balls et al. (1995)
Chlorhexidine	55-56-1	100%	Solid		water insoluble		3.00	Nonirritant	Moderate	Balls et al. (1995)
Chlorhexidine	55-56-1	100%	Solid		water insoluble		6.00	Moderate		Balls et al. (1995)
Chlorhexidine	55-56-1	100%	Solid		water insoluble		11.00	Moderate		Balls et al. (1995)
Dibenzyl phosphate	1623-08-1	100%	Solid	99.5	water insoluble		0.00	Nonirritant	Severe	Balls et al. (1995)
Dibenzyl phosphate	1623-08-1	100%	Solid	99.5	water insoluble		18.00	Severe		Balls et al. (1995)
Dibenzyl phosphate	1623-08-1	100%	Solid	99.5	water insoluble		0.00	Nonirritant		Balls et al. (1995)
Dibenzyl phosphate	1623-08-1	100%	Solid	99.5	water insoluble		15.00	Severe		Balls et al. (1995)
2,5-Dimethylhexanediol	110-03-2	100%	Solid	99.5	water insoluble		18.00	Severe	Severe	Balls et al. (1995)
2,5-Dimethylhexanediol	110-03-2	100%	Solid	99.5	water insoluble		18.00	Severe		Balls et al. (1995)
Fomesafen	72128-02-0	100%	Solid	97.5	water soluble		0.00	Nonirritant	Moderate	Balls et al. (1995)
Fomesafen	72128-02-0	100%	Solid	97.5	water soluble		9.00	Moderate		Balls et al. (1995)
Fomesafen	72128-02-0	100%	Solid	97.5	water soluble		6.00	Moderate		Balls et al. (1995)
Fomesafen	72128-02-0	100%	Solid	97.5	water soluble		6.00	Moderate		Balls et al. (1995)
Imidazole	288-32-4	100%	Solid	99	water soluble		18.00	Severe	Severe	Balls et al. (1995)
Imidazole	288-32-4	100%	Solid	99	water soluble		18.00	Severe		Balls et al. (1995)
Maneb	12427-38-2	100%	Solid	ca. 90	water soluble		0.00	Nonirritant	Nonirritant	Balls et al. (1995)

Substance Name	CASRN	*In Vitro* Concentration Tested	*In Vitro* Physical Form Tested	Purity (%)	Solubility[1]	pH	S-Score[2]	S-Score Classification	Overall S-Score Classification	Reference
1-Naphthalene acetic acid, Na salt	61-31-4	100%	Solid	99	water soluble		18.00	Severe	Severe	Balls et al. (1995)
1-Naphthalene acetic acid, Na salt	61-31-4	100%	Solid	99	water soluble		18.00	Severe		Balls et al. (1995)
1-Naphthalene acetic acid	86-87-3	100%	Solid	96	water insoluble		6.00	Moderate	Moderate	Balls et al. (1995)
1-Naphthalene acetic acid	86-87-3	100%	Solid	96	water insoluble		13.00	Moderate		Balls et al. (1995)
1-Naphthalene acetic acid	86-87-3	100%	Solid	96	water insoluble		0.00	Nonirritant		Balls et al. (1995)
1-Naphthalene acetic acid	86-87-3	100%	Solid	96	water insoluble		4.00	Nonirritant		Balls et al. (1995)
Potassium cyanate	590-28-3	100%	Solid	97	water soluble		18.00	Severe	Severe	Balls et al. (1995)
Promethazine HCl	58-33-3	100%	Solid	98	water soluble		18.00	Severe	Severe	Balls et al. (1995)
Promethazine HCl	58-33-3	100%	Solid	98	water soluble		18.00	Severe		Balls et al. (1995)
Quinacrine	69-05-6	100%	Solid		water soluble		0.00	Nonirritant	Nonirritant	Balls et al. (1995)
Quinacrine	69-05-6	100%	Solid		water soluble		4.00	Nonirritant		Balls et al. (1995)
Quinacrine	69-05-6	100%	Solid		water soluble		3.00	Nonirritant		Balls et al. (1995)
Sodium oxalate	62-76-0	100%	Solid	>99	water soluble		0.00	Nonirritant	Moderate	Balls et al. (1995)
Sodium oxalate	62-76-0	100%	Solid	>99	water soluble		12.00	Moderate		Balls et al. (1995)
Sodium oxalate	62-76-0	100%	Solid	>99	water soluble		11.00	Moderate		Balls et al. (1995)
Sodium oxalate	62-76-0	100%	Solid	>99	water soluble		9.00	Moderate		Balls et al. (1995)
Sodium perborate	10486-00-7	100%	Solid	98.6	water soluble		0.00	Nonirritant	Nonirritant	Balls et al. (1995)
Sodium perborate	10486-00-7	100%	Solid	98.6	water soluble		0.00	Nonirritant		Balls et al. (1995)
Sodium perborate	10486-00-7	100%	Solid	98.6	water soluble		7.00	Moderate		Balls et al. (1995)
Tetraaminopyrimidine sulfate	5392-28-9	100%	Solid	97	water insoluble		0.00	Nonirritant	Nonirritant	Balls et al. (1995)
Tetraaminopyrimidine sulfate	5392-28-9	100%	Solid	97	water insoluble		0.00	Nonirritant		Balls et al. (1995)
Tetraaminopyrimidine sulfate	5392-28-9	100%	Solid	97	water insoluble		6.00	Moderate		Balls et al. (1995)
Thiourea	62-56-6	100%	Solid	>99	water soluble		18.00	Severe	Severe	Balls et al. (1995)
Thiourea	62-56-6	100%	Solid	>99	water soluble		13.00	Moderate		Balls et al. (1995)

Abbreviation: CASRN = Chemical Abstract Service Registry Number, HCl = Hydrochloric acid.

[1] Solubility obtained from literature sources, where available expressed as g/mL

[2] S-Score represents irritation scores that were calculated using the method described in Balls et al. (1995)

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