

Substance Name	CASRN	Test Lab	<i>In Vitro</i> Concentration Tested	<i>In Vitro</i> 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)

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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)

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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-Chlorooctane-8-ol		AP	10%	Unknown		insoluble	n.s.	6.8	Moderate	Moderate	Spielmann et al. (1996)
1-Chlorooctane-8-ol		MD	10%	Unknown		insoluble	n.s.	4.3	Slight		Spielmann et al. (1996)

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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)

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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)

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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-Epoxyoctane	286-62-4	MD	10%	Solid		<2.5	4.5	np		Severe	Spielmann et al. (1996)
1,2-Epoxyoctane	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)

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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)

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Granufom	30525-89-4	BD	10%	Solid		250	4	2.9	Slight	Slight	Spielmann et al. (1996)
Granufom	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)

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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)

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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)

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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)
Isodecylglicoside		AP	10%	Unknown		readily soluble	9	17.2	Severe	Severe	Spielmann et al. (1996)
Isodecylglicoside		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	Severe	Spielmann et al. (1996)
L-Lysine Monohydrate	39665-12-8	BD	10%	Solid		1500	10	10	Severe		Spielmann et al. (1996)
L-Lysine Monohydrate	39665-12-8	HO	10%	Solid		1500	10	8.25	Moderate		Spielmann et al. (1996)

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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)

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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)

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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)

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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	<i>In Vitro</i> Concentration Tested	<i>In Vitro</i> 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)

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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)

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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)

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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)
Sodium pyrosulfite	7681-57-4	AP	10%	Solid		650	4.6	17.4	Severe	Severe	Spielmann et al. (1996)
Sodium pyrosulfite	7681-57-4	BD	10%	Solid		650	4.6	12.6	Severe		Spielmann et al. (1996)
Sodium pyrosulfite	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)
Trisooctylamine	25549-16-0	BG	10%	Solid		0.5	7	0.8	Nonirritant	Nonirritant	Spielmann et al. (1996)
Trisooctylamine	25549-16-0	MD	10%	Solid		0.5	7	0	Nonirritant		Spielmann et al. (1996)

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2,2,3-Trimethyl-3-Cyclopentene-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-Cyclopentene-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 Registry 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.