3T3 NRU Predictions: RC Rat-Only Weight Regression

RC Rat-Only Weight Regression: Log LD50 (mg/kg) = 0.372 log IC50 (ug/mL) + 2.024

Chemical[a]	Log Observed LD_{50} (mg/kg)[1]	3T3 Log IC_{50} (ug/mL)[2]	Log Predicted LD_{50} (mg/kg)[3]	Observed LD_{50} (mg/kg)[1]	3T3 IC_{50} (ug/mL)[2]	Predicted LD_{50} (mg/kg)[3]	Observed LD_{50} - Predicted LD_{50} (mg/kg)	Observed Toxicity Category[4] (mg/kg)	Predicted Toxicity Category[4] (mg/kg)
Acetaminophen	3.33	1.68	2.65	2162	47.7	445	1717	2000-5000	300-2000
Acetonitrile	3.56	3.90	3.47	3595	7951	2985	610	2000-5000	2000-5000
Acetylsalicylic acid	3.18	2.83	3.08	1506	676	1194	312	300-2000	300-2000
Aminopterin	0.845	-2.20	1.20	7.00	0.006	16.0	-9.00	5-50	5-50
5-Aminosalicylic acid	3.54	3.22	3.22	3428	1667	1669	1759	2000-5000	300-2000
Arsenic III trioxide	1.40	0.293	2.13	25.1	1.96	136	-111	5-50	50-300
Boric acid	3.53	3.27	3.24	3426	1850	1735	1691	2000-5000	300-2000
Busulfan	1.08	1.89	2.73	12.1	77.7	534	-521	5-50	300-2000
Cadmium II chloride	2.13	-0.286	1.92	135	0.518	82.7	52.5	50-300	50-300
Chloramphenicol	3.54	2.11	2.81	3490	128	643	2847	2000-5000	300-2000
Citric acid	3.77	2.90	3.10	5929	796	1268	4661	> 5000	300-2000
Cupric sulfate pentahydrate	2.68	1.62	2.63	475	42.1	425	50.1	300-2000	300-2000
Cycloheximide	0.301	-0.727	1.75	2.00	0.187	56.7	-54.7	< 5	50-300
Dibutyl phthalate	3.95	1.70	2.66	8892	49.7	452	8440	> 5000	300-2000
Diethyl phthalate	3.97	2.03	2.78	9311	107	602	8709	> 5000	300-2000
Digoxin	1.45	2.67	3.02	28.3	466	1039	-1010	5-50	300-2000
Dimethylformamide	3.72	3.72	3.41	5305	5224	2553	2752	> 5000	2000-5000
Diquat dibromide monohydrate	2.20	0.905	2.36	160	8.04	229	-69.5	50-300	50-300
Ethanol	4.05	3.81	3.44	11324	6523	2773	8551	> 5000	2000-5000
Ethylene glycol	3.85	4.39	3.66	7161	24317	4524	2637	> 5000	2000-5000
Gibberellic acid	3.78	3.89	3.47	6039	7810	2965	3074	> 5000	2000-5000
Glycerol	4.30	4.39	3.66	19770	24655	4548	15222	> 5000	2000-5000
Hexachlorophene	1.91	0.623	2.26	82.0	4.19	180	-98.2	50-300	50-300
Lactic acid	3.56	3.48	3.32	3635	3044	2089	1546	2000-5000	2000-5000
Lithium I carbonate	2.77	2.75	3.05	590	562	1114	-524	300-2000	300-2000
Meprobamate	3.14	2.72	3.03	1387	519	1081	305	300-2000	300-2000
Mercury II chloride	1.60	0.615	2.25	40.2	4.12	179	-139	5-50	50-300
Phenol	2.74	1.82	2.70	548	66.3	503	44.6	300-2000	300-2000
Phenylthiourea	0.477	1.90	2.73	3.00	79.0	537	-534	< 5	300-2000
Potassium I chloride	3.45	3.55	3.34	2802	3551	2212	590.2	2000-5000	2000-5000

3T3 NRU Predictions: RC Rat-Only Weight Regression

Chemical[a]	Log Observed LD_{50} (mg/kg)[1]	3T3 Log IC_{50} (ug/mL)[2]	Log Predicted LD_{50} (mg/kg)[3]	Observed LD_{50} (mg/kg)[1]	3T3 IC_{50} (ug/mL)[2]	Predicted LD_{50} (mg/kg)[3]	Observed LD_{50} - Predicted LD_{50} (mg/kg)	Observed Toxicity Category[4] (mg/kg)	Predicted Toxicity Category[4] (mg/kg)
2-Propanol	3.71	3.56	3.35	5105	3618	2227	2878	> 5000	2000-5000
Propranolol HCl	2.67	1.14	2.45	466	14	281	185	300-2000	50-300
Sodium arsenite	1.64	-0.120	1.98	43.6	0.759	95.4	-51.8	5-50	50-300
Sodium chloride	3.61	3.67	3.39	4050	4730	2461	1589	2000-5000	2000-5000
Sodium dichromate dihydrate	1.70	-0.232	1.94	50.5	0.587	86.7	-36.2	50-300	50-300
Sodium hypochlorite	4.01	3.04	3.16	10328	1103	1431	8896	> 5000	300-2000
Sodium I fluoride	2.10	1.89	2.73	127	78.0	534	-408	50-300	300-2000
Sodium oxalate	2.80	1.58	2.61	633	37.7	408	225	300-2000	300-2000
Sodium selenate	0.477	1.46	2.57	3.00	29.0	370	-367	< 5	300-2000
Thallium I sulfate	1.40	0.759	2.31	25.0	5.74	202	-177	5-50	50-300
Trichloroacetic acid	3.72	2.96	3.12	5229	902	1328	3900	> 5000	300-2000
1,1,1-Trichloroethane	4.08	4.24	3.60	12078	17248	3982	8096	> 5000	2000-5000
Triethylenemelamine	0.602	-0.565	1.81	4.00	0.272	65.1	-61.1	< 5	50-300
Triphenyltin Hydroxide	2.52	-1.76	1.37	329	0.017	23.3	306	300-2000	5-50
Valproic acid	3.00	2.96	3.13	996	916	1336	-340	300-2000	300-2000
Xylene	3.67	2.86	3.09	4665	721	1222	3443	2000-5000	300-2000

[a]Three chemicals were excluded because no rat LD_{50} was identified: epinephrine bitartrate, colchicine, and propylparaben. Carbon tetrachloride and methanol were excluded because an IC_{50} value could not be determined. Twenty-one chemicals were excluded based on their mechanisms of action: amitriptyline HCl, atropine sulfate, caffeine, carbamazepine, chloral hydrate, dichlorvos , disulfoton, endosulfan, fenpropathrin, glutethimide, haloperidol, lindane, nicotine, paraquat, parathion, phenobarbital, physostigmine, potassium cyanide, procainamide HCl, strychnine, and verapamil HCl (see **Section 6, Table 6-3**).

[1] reference LD_{50} values that were collected from the literature

[2] combined 3T3 IC_{50} values from three laboratories

[3] LD_{50} determined using: $\log LD_{50}$ (mg/kg) = 0.372 $\log IC_{50}$ ug/mL + 2.024

[4]Globally Harmonized System (GHS) hazard classification:

Category	Oral LD_{50} Limits
1	$LD_{50} \leq 5$ mg/kg
2	$5 < LD_{50} \leq 50$ mg/kg
3	$50 < LD_{50} \leq 300$ mg/kg
4	$300 < LD_{50} \leq 2000$ mg/kg
5	$2000 < LD_{50} \leq 5000$ mg/kg
Unclassified	$LD_{50} > 5000$ mg/kg