3T3 NRU Predictions: RC Rat-Only Weight Regression
Log LD_{50} (mg/kg) = 0.372 log IC_{50} (ug/mL) + 2.024

Reference Substance[1]	Log Reference LD_{50} (mg/kg)[2]	Reference LD_{50} (mg/kg)[2]	Observed Toxicity Category[3] (mg/kg)	Log Predicted LD_{50} (mg/kg)[4]	Predicted LD_{50} (mg/kg)[5]	Predicted Toxicity Category[3] (mg/kg)	3T3 Log IC_{50} (ug/mL)[6]
1,1,1-Trichloroethane	4.082	12078	>5000	3.628	5078	>5000	4.311
2-Propanol	3.708	5105	>5000	3.342	1494	300-2000	3.543
5-Aminosalicylic Acid	3.535	3428	2000-5000	3.223	1825	300-2000	3.222
Acetaminophen	3.335	2162	2000-5000	2.648	381	300-2000	1.678
Acetonitrile	3.556	3595	2000-5000	3.475	1731	300-2000	3.900
Acetylsalicylic Acid	3.178	1506	300-2000	3.077	1346	300-2000	2.830
Aminopterin	0.845	7	5-50	1.207	14	5-50	-2.195
Amitriptyline HCl	2.543	349	300-2000	2.340	248	50-300	0.848
Arsenictrioxide	1.400	25	5-50	2.142	112	50-300	0.316
Atropine Sulfate	2.913	819	300-2000	2.724	1099	300-2000	1.881
Boric Acid	3.535	3426	2000-5000	3.239	1149	300-2000	3.267
Busulfan	1.084	12	5-50	2.727	620	300-2000	1.890
Cadmium chloride	2.131	135	50-300	1.918	58	50-300	-0.286
Caffeine	2.491	310	300-2000	2.836	730	300-2000	2.183
Carbamazepine	3.448	2807	2000-5000	2.773	686	300-2000	2.014
Chloral Hydrate	2.805	638	300-2000	2.866	723	300-2000	2.263
Chloramphenicol	3.543	3490	2000-5000	2.811	906	300-2000	2.115
Citric Acid	3.773	5929	>5000	3.097	1472	300-2000	2.884
Cupric Sulfate Pentahydrate	2.677	475	300-2000	2.610	455	300-2000	1.576
Cycloheximide	0.301	2	<5	1.753	47	5-50	-0.727
Dibutyl Phthalate	3.949	8892	>5000	2.633	514	300-2000	1.637
Dichlorvos (DDVP)	1.769	59	50-300	2.489	305	300-2000	1.249
Diethyl Phthalate	3.969	9311	>5000	2.779	674	300-2000	2.031
Digoxin	1.451	28	5-50	3.009	2550	2000-5000	2.649
Dimethylformamide	3.725	5305	>5000	3.407	1990	300-2000	3.718
Diquat Dibromide Monohydrate	2.204	160	50-300	2.361	284	50-300	0.905
Disulfoton	0.699	5	<5	2.992	1352	300-2000	2.602
Endosulfan	1.444	28	5-50	2.310	265	50-300	0.770
Ethanol	4.054	11324	>5000	3.443	1693	300-2000	3.814
Ethyleneglycol	3.855	7161	>5000	3.656	3574	2000-5000	4.388
Fenpropathrin	1.879	76	50-300	2.533	445	300-2000	1.368
Gibberellic Acid	3.781	6039	>5000	3.472	5683	>5000	3.893
Glutethimide	2.778	600	300-2000	2.864	838	300-2000	2.258
Glycerol	4.296	19770	>5000	3.656	4452	2000-5000	4.386
Haloperidol	2.519	330	300-2000	2.317	258	50-300	0.787
Hexachlorophene	1.914	82	50-300	2.256	228	50-300	0.623
Lactic Acid	3.561	3635	2000-5000	3.320	1765	300-2000	3.483
Lindane	2.000	100	50-300	2.786	798	300-2000	2.047
Lithium carbonate	2.771	590	300-2000	3.047	752	300-2000	2.749
Meprobamate	3.142	1387	300-2000	3.025	1301	300-2000	2.690
Mercury Chloride	1.604	40	5-50	2.253	180	50-300	0.615
Nicotine	1.843	70	50-300	2.975	963	300-2000	2.557

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Reference Substance[1]	Log Reference LD_{50} (mg/kg)[2]	Reference LD_{50} (mg/kg)[2]	Observed Toxicity Category[3] (mg/kg)	Log Predicted LD_{50} (mg/kg)[4]	Predicted LD_{50} (mg/kg)[5]	Predicted Toxicity Category[3] (mg/kg)	3T3 Log IC_{50} (ug/mL)[6]
Paraquat	1.967	93	50-300	2.509	351	300-2000	1.304
Parathion	0.785	6	5-50	2.609	494	300-2000	1.573
Phenobarbital	2.350	224	50-300	3.054	1457	300-2000	2.768
Phenol	2.739	548	300-2000	2.702	337	300-2000	1.822
Phenylthiourea	0.477	3	<5	2.730	477	300-2000	1.898
Physostigmine	0.699	5	<5	2.554	412	300-2000	1.425
Potassium Cyanide	0.857	7	5-50	2.597	206	50-300	1.540
Potassium chloride	3.447	2802	2000-5000	3.345	1699	300-2000	3.551
Procainamide HCl	3.290	1950	300-2000	3.008	1404	300-2000	2.644
Propranolol	2.668	466	300-2000	2.452	325	300-2000	1.150
Sodium Arsenite	1.639	44	5-50	1.979	57	50-300	-0.120
Sodium Chloride	3.607	4050	2000-5000	3.392	1683	300-2000	3.676
Sodium Dichromate Dihydrate	1.703	50	50-300	1.938	81	50-300	-0.232
Sodium Hypochlorite	4.014	10328	>5000	3.146	990	300-2000	3.017
Sodium Oxalate	2.801	633	300-2000	2.608	319	300-2000	1.570
Sodium fluoride	2.103	127	50-300	2.728	230	50-300	1.892
Sodium selenate	0.477	3	<5	2.568	347	300-2000	1.463
Strychnine	0.799	6	5-50	2.842	1005	300-2000	2.198
Thallium Sulfate	1.398	25	5-50	2.297	288	50-300	0.735
Trichloroacetic Acid	3.718	5229	>5000	3.123	1445	300-2000	2.955
Triethylenemelamine	0.602	4	<5	1.814	47	5-50	-0.565
Triphenyltin Hydroxide	2.517	329	300-2000	1.368	19	5-50	-1.764
Valproic Acid	2.998	996	300-2000	3.109	1296	300-2000	2.917
Verapamil HCl	2.045	111	50-300	2.598	643	300-2000	1.543
Xylene	3.669	4665	2000-5000	3.087	1028	300-2000	2.858

[1]Three chemicals were excluded because no rat oral LD_{50} was identified: epinephrine bitartrate, colchicine, and propylparaben. Carbon tetrachloride and methanol were excluded because IC_{50} values could not be determined.
[2]Reference LD_{50} in mmol/kg from **Table 4-2**. Reference rat oral LD_{50} values were developed from rat acute oral LD_{50} studies located using literature searches, secondary references, and electronic database searches.
[3]Globally Harmonized System (GHS) hazard classification (UN 2005):

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

[4]LD_{50} determined using NRU IC_{50} in RC rat-only weight regression: Log LD_{50} (mg/kg) = 0.372 log IC_{50} (ug/mL) + 2.024
[5]LD_{50} in mg/kg (converted from results of RC rat-only weight regression)
[6]Combined 3T3 IC_{50} values from three laboratories