3T3 NRU Predictions: RC Rat-Only Millimole Regression
Log LD_{50} (mmol/kg) = 0.439 log IC_{50} (mM) + 0.621

Reference Substance[1]	Log Reference LD_{50} (mmol/kg)[2]	Reference LD_{50} (mg/kg)[2]	Observed Toxicity Category[3] (mg/kg)	Log Predicted LD_{50} (mmol/kg)[4]	Predicted LD_{50} (mg/kg)[5]	Predicted Toxicity Category[3] (mg/kg)	3T3 Log IC_{50} (mM)[6]
1,1,1-Trichloroethane	1.957	12078	>5000	1.580	5078	>5000	2.186
2-Propanol	1.929	5105	>5000	1.395	1494	300-2000	1.764
5-Aminosalicylic Acid	1.350	3428	2000-5000	1.076	1825	300-2000	1.037
Acetaminophen	1.155	2162	2000-5000	0.401	381	300-2000	-0.501
Acetonitrile	1.942	3595	2000-5000	1.625	1731	300-2000	2.287
Acetylsalicylic Acid	0.922	1506	300-2000	0.873	1346	300-2000	0.574
Aminopterin	-1.799	7	5-50	-1.504	14	5-50	-4.839
Amitriptyline HCl	0.046	349	300-2000	-0.103	248	50-300	-1.648
Arsenictrioxide	-0.897	25	5-50	-0.248	112	50-300	-1.980
Atropine Sulfate	0.071	819	300-2000	0.199	1099	300-2000	-0.961
Boric Acid	1.744	3426	2000-5000	1.269	1149	300-2000	1.476
Busulfan	-1.308	12	5-50	0.401	620	300-2000	-0.501
Cadmium chloride	-0.132	135	50-300	-0.498	58	50-300	-2.549
Caffeine	0.203	310	300-2000	0.575	730	300-2000	-0.105
Carbamazepine	1.075	2807	2000-5000	0.463	686	300-2000	-0.360
Chloral Hydrate	0.586	638	300-2000	0.640	723	300-2000	0.044
Chloramphenicol	1.033	3490	2000-5000	0.448	906	300-2000	-0.395
Citric Acid	1.489	5929	>5000	0.884	1472	300-2000	0.600
Cupric Sulfate Pentahydrate	0.279	475	300-2000	0.260	455	300-2000	-0.822
Cycloheximide	-2.148	2	<5	-0.774	47	5-50	-3.177
Dibutyl Phthalate	1.504	8892	>5000	0.267	514	300-2000	-0.807
Dichlorvos (DDVP)	-0.576	59	50-300	0.140	305	300-2000	-1.095
Diethyl Phthalate	1.622	9311	>5000	0.482	674	300-2000	-0.316
Digoxin	-1.441	28	5-50	0.514	2550	2000-5000	-0.244
Dimethylformamide	1.861	5305	>5000	1.435	1990	300-2000	1.854
Diquat Dibromide Monohydrate	-0.355	160	50-300	-0.105	284	50-300	-1.654
Disulfoton	-1.739	5	<5	0.693	1352	300-2000	0.163
Endosulfan	-1.165	28	5-50	-0.187	265	50-300	-1.840
Ethanol	2.391	11324	>5000	1.565	1693	300-2000	2.151
Ethylene glycol	2.062	7161	>5000	1.760	3574	2000-5000	2.595
Fenpropathrin	-0.664	76	50-300	0.105	445	300-2000	-1.175
Gibberellic Acid	1.241	6039	>5000	1.215	5683	>5000	1.353
Glutethimide	0.441	600	300-2000	0.586	838	300-2000	-0.079
Glycerol	2.332	19770	>5000	1.684	4452	2000-5000	2.422
Haloperidol	-0.057	330	300-2000	-0.164	258	50-300	-1.788
Hexachlorophene	-0.696	82	50-300	-0.251	228	50-300	-1.987
Lactic Acid	1.606	3635	2000-5000	1.292	1765	300-2000	1.529
Lindane	-0.464	100	50-300	0.438	798	300-2000	-0.416
Lithium carbonate	0.902	590	300-2000	1.008	752	300-2000	0.881
Meprobamate	0.803	1387	300-2000	0.775	1301	300-2000	0.351
Mercury Chloride	-0.830	40	5-50	-0.177	180	50-300	-1.819
Nicotine	-0.367	70	50-300	0.774	963	300-2000	0.347

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Reference Substance[1]	Log Reference LD_{50} (mmol/kg)[2]	Reference LD_{50} (mg/kg)[2]	Observed Toxicity Category[3] (mg/kg)	Log Predicted LD_{50} (mmol/kg)[4]	Predicted LD_{50} (mg/kg)[5]	Predicted Toxicity Category[3] (mg/kg)	3T3 Log IC_{50} (mM)[6]
Paraquat	-0.443	93	50-300	0.135	351	300-2000	-1.106
Parathion	-1.679	6	5-50	0.230	494	300-2000	-0.891
Phenobarbital	-0.016	224	50-300	0.798	1457	300-2000	0.402
Phenol	0.765	548	300-2000	0.554	337	300-2000	-0.152
Phenylthiourea	-1.705	3	<5	0.496	477	300-2000	-0.285
Physostigmine	-1.741	5	<5	0.175	412	300-2000	-1.015
Potassium Cyanide	-0.956	7	5-50	0.501	206	50-300	-0.274
Potassium chloride	1.575	2802	2000-5000	1.358	1699	300-2000	1.678
Procainamide HCl	0.856	1950	300-2000	0.713	1404	300-2000	0.210
Propranolol	0.197	466	300-2000	0.041	325	300-2000	-1.321
Sodium Arsenite	-0.474	44	5-50	-0.360	57	50-300	-2.234
Sodium Chloride	1.841	4050	2000-5000	1.459	1683	300-2000	1.910
Sodium Dichromate Dihydrate	-0.771	50	50-300	-0.567	81	50-300	-2.706
Sodium Hypochlorite	2.142	10328	>5000	1.124	990	300-2000	1.145
Sodium Oxalate	0.674	633	300-2000	0.376	319	300-2000	-0.557
Sodium fluoride	0.480	127	50-300	0.739	230	50-300	0.269
Sodium selenate	-1.799	3	<5	0.264	347	300-2000	-0.814
Strychnine	-1.725	6	5-50	0.478	1005	300-2000	-0.326
Thallium Sulfate	-1.305	25	5-50	-0.243	288	50-300	-1.968
Trichloroacetic Acid	1.505	5229	>5000	0.947	1445	300-2000	0.742
Triethylenemelamine	-1.708	4	<5	-0.641	47	5-50	-2.875
Triphenyltin Hydroxide	-0.047	329	300-2000	-1.279	19	5-50	-4.329
Valproic Acid	0.839	996	300-2000	0.954	1296	300-2000	0.758
Verapamil HCl	-0.646	111	50-300	0.117	643	300-2000	-1.148
Xylene	1.643	4665	2000-5000	0.986	1028	300-2000	0.832

[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 millimole regression: Log LD_{50} (mmol/kg) = 0.439 log IC_{50} (mM) + 0.621.
[5]LD_{50} in mg/kg (converted from results of RC rat-only millimole regression).
[6]Combined 3T3 IC_{50} values from three laboratories.