NHK 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)	NHK Log IC_{50} (mM)[6]
1,1,1-Trichloroethane	1.957	12078	>5000	3.478	3009	2000-5000	1.784
2-Propanol	1.929	5105	>5000	3.411	2579	300-2000	1.951
5-Aminosalicylic Acid	1.350	3428	2000-5000	2.645	442	300-2000	-0.516
Acetaminophen	1.155	2162	2000-5000	3.034	1081	300-2000	0.535
Acetonitrile	1.942	3595	2000-5000	3.505	3196	300-2000	2.367
Acetylsalicylic Acid	0.922	1506	300-2000	3.059	1145	300-2000	0.526
Aminopterin	-1.799	7	5-50	3.073	1184	5-50	0.177
Amitriptyline HCl	0.046	349	300-2000	2.378	239	50-300	-1.545
Arsenictrioxide	-0.897	25	5-50	2.335	216	50-300	-1.461
Atropine Sulfate	0.071	819	300-2000	2.736	544	300-2000	-0.929
Boric Acid	1.744	3426	2000-5000	3.000	1001	300-2000	0.833
Busulfan	-1.308	12	5-50	2.922	836	300-2000	0.024
Cadmium chloride	-0.132	135	50-300	2.119	131	50-300	-2.009
Caffeine	0.203	310	300-2000	3.067	1168	300-2000	0.516
Carbamazepine	1.075	2807	2000-5000	2.738	547	300-2000	-0.453
Chloral Hydrate	0.586	638	300-2000	2.814	652	300-2000	-0.094
Chloramphenicol	1.033	3490	2000-5000	2.968	929	300-2000	0.028
Citric Acid	1.489	5929	>5000	2.997	992	300-2000	0.331
Cupric Sulfate Pentahydrate	0.279	475	300-2000	2.877	754	300-2000	-0.104
Cycloheximide	-2.148	2	<5	1.602	40	5-50	-3.584
Dibutyl Phthalate	1.504	8892	>5000	2.566	368	300-2000	-0.987
Dichlorvos (DDVP)	-0.576	59	50-300	2.407	255	50-300	-1.315
Diethyl Phthalate	1.622	9311	>5000	2.798	628	300-2000	-0.266
Digoxin	-1.441	28	5-50	0.909	8	5-50	-5.889
Dimethylformamide	1.861	5305	>5000	3.471	2958	2000-5000	2.026
Diquat Dibromide Monohydrate	-0.355	160	50-300	2.261	182	50-300	-1.922
Disulfoton	-1.739	5	<5	2.928	848	300-2000	-0.007
Endosulfan	-1.165	28	5-50	2.146	140	50-300	-2.282
Ethanol	2.391	11324	>5000	3.512	3253	2000-5000	2.337
Ethyleneglycol	2.062	7161	>5000	3.744	5549	2000-5000	2.831
Fenpropathrin	-0.664	76	50-300	2.167	147	50-300	-2.158
Gibberellic Acid	1.241	6039	>5000	3.310	2040	2000-5000	0.916
Glutethimide	0.441	600	300-2000	2.857	720	300-2000	-0.098
Glycerol	2.332	19770	>5000	3.658	4553	2000-5000	2.429
Haloperidol	-0.057	330	300-2000	2.220	166	50-300	-2.049
Hexachlorophene	-0.696	82	50-300	1.451	28	5-50	-4.149
Lactic Acid	1.606	3635	2000-5000	3.183	1524	300-2000	1.161
Lindane	-0.464	100	50-300	2.497	314	300-2000	-1.191
Lithium carbonate	0.902	590	300-2000	3.017	1040	300-2000	0.801
Meprobamate	0.803	1387	300-2000	2.973	941	300-2000	0.213
Mercury Chloride	-0.830	40	5-50	2.308	203	50-300	-1.671
Methanol	2.434	8710	>5000	3.209	1616	300-2000	1.679
Nicotine	-0.367	70	50-300	2.778	600	300-2000	-0.182

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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)	NHK Log IC_{50} (mM)[6]
Paraquat	-0.443	93	50-300	2.690	489	300-2000	-0.621
Parathion	-1.679	6	5-50	2.575	376	300-2000	-0.983
Phenobarbital	-0.016	224	50-300	3.010	1024	300-2000	0.285
Phenol	0.765	548	300-2000	2.722	527	300-2000	-0.098
Phenylthiourea	-1.705	3	<5	2.964	920	300-2000	0.344
Physostigmine	-1.741	5	<5	2.748	560	300-2000	-0.493
Potassium Cyanide	-0.956	7	5-50	2.568	370	50-300	-0.352
Potassium chloride	1.575	2802	2000-5000	3.270	1862	300-2000	1.477
Procainamide HCl	0.856	1950	300-2000	3.230	1697	2000-5000	0.807
Propranolol	0.197	466	300-2000	2.604	402	300-2000	-0.912
Sodium Arsenite	-0.474	44	5-50	1.904	80	5-50	-2.435
Sodium Chloride	1.841	4050	2000-5000	3.252	1786	300-2000	1.534
Sodium Dichromate Dihydrate	-0.771	50	50-300	1.969	93	50-300	-2.622
Sodium Hypochlorite	2.142	10328	>5000	3.206	1606	300-2000	1.305
Sodium Oxalate	0.674	633	300-2000	2.965	923	300-2000	0.404
Sodium fluoride	0.480	127	50-300	2.652	449	50-300	0.066
Sodium selenate	-1.799	3	<5	2.399	251	50-300	-1.267
Strychnine	-1.725	6	5-50	2.687	486	300-2000	-0.743
Thallium Sulfate	-1.305	25	5-50	1.719	52	50-300	-3.522
Trichloroacetic Acid	1.505	5229	>5000	2.997	994	300-2000	0.403
Triethylenemelamine	-1.708	4	<5	2.124	133	50-300	-2.042
Triphenyltin Hydroxide	-0.047	329	300-2000	1.281	19	5-50	-4.562
Valproic Acid	0.839	996	300-2000	3.032	1076	300-2000	0.550
Verapamil HCl	-0.646	111	50-300	2.702	503	300-2000	-0.869
Xylene	1.643	4665	2000-5000	3.016	1039	300-2000	0.642

[1]Three chemicals were excluded because no rat oral LD_{50} was identified: epinephrine bitartrate, colchicine, and propylparaben. Carbon tetrachloride was 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 NHK IC_{50} values from three laboratories