

**In Vivo and In Vitro Data Comparison
Sorted by Substance**

Substance/Product Name	CASRN	Concentration Tested	In Vitro Classification (GHS)	In Vivo Classification (GHS)	In Vitro Classification (EPA)	In Vivo Classification (EPA)	In Vitro Classification (EU)	In Vivo Classification (EU)	Reference
Acetaldehyde	75-07-0	undiluted	2A	-	II	-	R36	R36	Prinsen and Koeter (1993)
Acetic acid	64-19-7	10%	1	1	I	I	R41	R41	Prinsen and Koeter (1993)
Acetone	67-64-1	undiluted	2A	2A	II	II	R36	R36	Balls et al. (1995)
Ammonium nitrate	6484-52-2	undiluted	2B	2B	III	III	NI	R36	Balls et al. (1995)
L-Aspartic acid	70-47-3	neat	2A	SCNM	II	SCNM	R36	SCNM	Balls et al. (1995)
Benzalkonium chloride (1%)	8001-54-5	1%	2A	1	II	I	R36	R41	Balls et al. (1995)
Benzalkonium chloride (5%)	8001-54-5	5%	1	1	I	I	R41	R41	Balls et al. (1995)
Benzalkonium chloride (10%)	8001-54-5	10%	1	1	I	I	R41	R41	Balls et al. (1995)
Benzalkonium chloride (100%)	8001-54-5	undiluted	1	1	I	I	R41	R41	Prinsen and Koeter (1993)
Brij 35	9002-92-0	undiluted	NI	-	IV	-	NI	NI	Prinsen and Koeter (1993)
1-Butanol	71-36-3	undiluted	1	2A	I	II	R41	R41	Prinsen and Koeter (1993)
2-Butoxyethyl acetate	112-07-2	undiluted	2B	-	III	-	NI	NI	Prinsen and Koeter (1993)
n-Butyl acetate	123-86-4	undiluted	2A	NI	II	III	R36	NI	Balls et al. (1995)
gamma-Butyrolactone	96-48-0	undiluted	2A	2A	II	II	R36	R36	Balls et al. (1995)
Captan 90 concentrate	133-06-2	neat	2B	1	III	I	NI	R41	Balls et al. (1995)
4-Carboxybenzaldehyde	619-66-9	neat	NI	2A	IV	II	NI	R36	Balls et al. (1995)
4-Carboxybenzaldehyde	619-66-9	neat	NI	2A	IV	II	NI	R36	Balls et al. (1995)
Cetylpyridinium bromide (0.1%)	140-72-7	0.1%	2B	NI	III	III	NI	NI	Balls et al. (1995)
Cetylpyridinium bromide (6%)	140-72-7	6%	2A	1	II	SCNM	R36	R41	Balls et al. (1995)
Cetylpyridinium bromide (6%)	140-72-7	undiluted	1	1	I	SCNM	R41	R41	Prinsen (2000)
Cetylpyridinium bromide (10%)	140-72-7	10%	2A	1	II	I	R36	R41	Balls et al. (1995)
Chlorhexidine	55-56-1	neat	1	1	I	SCNM	R41	SCNM	Balls et al. (1995)
Chloroform	67-66-3	undiluted	2A	-	II	-	R36	R36	Prinsen and Koeter (1993)
Cyclohexanol	108-93-0	undiluted	1	1	I	I	R41	R41	Balls et al. (1995)
Cyclohexylamino-functional PMS	—	undiluted	2A	-	II	-	R36	R36	Prinsen (2000)
Decamethylcyclopentasiloxane	—	undiluted	NI	-	NI	-	NI	NI	Prinsen (2000)
Dibenzoyl-L-tartaric acid	2743-38-6	neat	1	1	I	SCNM	R41	R41	Balls et al. (1995)
Dibenzyl phosphate	1623-08-1	neat	2A/2B	2A	II/III	II	R36	R36	Balls et al. (1995)
Dibutyltin dichloride	683-18-1	undiluted	1	-	I	-	R41	R41	Prinsen and Koeter (1993)
2,6-Dichlorobenzoyl chloride	4659-45-4	undiluted	2A	2A	II	II	R36	SCNM	Balls et al. (1995)
2,2-Dimethylbutanoic acid	595-37-9	undiluted	1	SCNM	I	I	R41	SCNM	Balls et al. (1995)
2,5-Dimethylhexanediol	110-03-2	neat	2B	1	III	I	R36	R41	Balls et al. (1995)
Dimethyl sulfoxide	67-68-5	undiluted	NI	2B	IV	III	NI	NI	Prinsen and Koeter (1993)
Ethanol	64-17-5	undiluted	1	2A	I	III	R41	NI	Balls et al. (1995)
Ethyl acetate	141-78-6	undiluted	2A	NI	II	III	R36	NI	Balls et al. (1995)
2-Ethyl-1-hexanol	104-76-7	undiluted	2A	2A	II	II	R36	R36	Balls et al. (1995)
Ethyl-2-methylacetoacetate	609-14-3	undiluted	2B	2B	III	III	NI	NI	Balls et al. (1995)
Ethyl trimethyl acetate	3938-95-2	undiluted	2B	NI	III	III	NI	NI	Balls et al. (1995)
Fomesafen	72128-02-0	neat	2B	NI	III	III	NI	NI	Balls et al. (1995)
Glycerol	56-81-5	undiluted	NI	NI	IV	IV	NI	NI	Prinsen and Koeter (1993)
n-Hexane	110-54-3	undiluted	NI	NI	IV	IV	NI	NI	Prinsen and Koeter (1993)
n-Hexanol	111-27-3	undiluted	1	2A	I	II	R41	R36	Balls et al. (1995)

**In Vivo and In Vitro Data Comparison
Sorted by Substance**

Substance/Product Name	CASRN	Concentration Tested	In Vitro Classification (GHS)	In Vivo Classification (GHS)	In Vitro Classification (EPA)	In Vivo Classification (EPA)	In Vitro Classification (EU)	In Vivo Classification (EU)	Reference
Imidazole	288-32-4	neat	1	1	I	I	R41	R41	Balls et al. (1995)
Isobutanol	78-83-1	undiluted	1	2A	I	II	R41	R36	Balls et al. (1995)
Isopropanol	67-63-0	undiluted	1	2A	I	III	R41	SCNM	Balls et al. (1995)
Maneb	12427-38-2	neat	NI	SCNM	IV	III	NI	SCNM	Balls et al. (1995)
Mercury (II) chloride	7487-94-7	undiluted	1	-	I	-	R41	R41	Prinsen and Koëter (1993)
2-Methoxyethanol	109-86-4	undiluted	2A	-	II	-	R36	R36	Prinsen and Koëter (1993)
Methyl acetate	79-20-9	undiluted	1	2A	I	II	R41	R36	Balls et al. (1995)
Methyl cyanoacetate	105-34-0	undiluted	NI	2A	IV	II	NI	R36	Balls et al. (1995)
Methylcyclopentane	96-37-7	undiluted	NI	NI	IV	III	NI	NI	Balls et al. (1995)
Methyl ethyl ketone	78-93-3	undiluted	1	2A	I	III	R41	R36	Balls et al. (1995)
Methyl isobutyl ketone	108-10-1	undiluted	2A	NI	II	III	R36	NI	Balls et al. (1995)
1-Naphthaleneacetic acid	86-87-3	neat	2B	1	III	I	R36	SCNM	Balls et al. (1995)
1-Naphthaleneacetic acid, sodium salt	61-31-4	neat	1	1	I	I	R41	R41	Balls et al. (1995)
n-Octanol	111-87-5	undiluted	2A	2B	II	II	R36	R36	Balls et al. (1995)
Parafluoraniiline	371-40-4	undiluted	1	SCNM	I	SCNM	R41	SCNM	Balls et al. (1995)
Polyethylene glycol 400	25322-68-3	undiluted	2B	NI	III	IV	R36	NI	Balls et al. (1995)
Potassium cyanate	590-28-3	neat	2B	SCNM	III	SCNM	R36	SCNM	Balls et al. (1995)
Potassium cyanate	590-28-3	neat	2B	SCNM	III	SCNM	R36	SCNM	Balls et al. (1995)
Promethazine HCl	58-33-3	neat	1	1	I	I	R41	R41	Balls et al. (1995)
Pyridine	110-86-1	undiluted	1	1	I	I	R41	R41	Balls et al. (1995)
Quinacrine	69-05-6	neat	2B	1	III	I	NI	R41	Balls et al. (1995)
Silver (I) nitrate	7761-88-8	3%	2B	-	III	-	NI	NI	Prinsen and Koëter (1993)
Sodium dodecyl sulfate	151-21-3	undiluted	2B	-	III	-	R41	R41	Prinsen and Koëter (1993)
Sodium fluorescein	518-47-8	20%	NI	-	IV	-	NI	NI	Prinsen and Koëter (1993)
Sodium hydroxide	1310-73-2	1%	1	1	I	I	R41	R41	Prinsen and Koëter (1993)
Sodium hydroxide (1%)	1310-73-2	1%	2A	2B	II	III	R36	R36	Balls et al. (1995)
Sodium hydroxide (10%)	1310-73-2	10%	1	1	I	I	R41	R41	Balls et al. (1995)
Sodium lauryl sulfate (3%)	151-21-3	3%	2B	NI	III	III	NI	NI	Balls et al. (1995)
Sodium lauryl sulfate (15%)	151-21-3	15%	2B	1	III	I	R36	R36	Balls et al. (1995)
Sodium oxalate	62-76-0	neat	2B	1	III	I	NI	R41	Balls et al. (1995)
Sodium perborate, 4H ₂ O	10486-00-7	neat	2B	1	III	I	NI	R41	Balls et al. (1995)
Tetraaminopyrimidine sulfate	5392-28-9	neat	2B	NI	III	III	NI	NI	Balls et al. (1995)
TNO-01 (Formulation-1)	n.p.	undiluted	NI	NI	IV	IV	NI	NI	Prinsen (1996)
TNO-02 (Formulation-2)	n.p.	undiluted	2A	2A	II	II	R36	R36	Prinsen (1996)
TNO-03 (Pesticide-1)	n.p.	undiluted	NI	NI	IV	III	NI	NI	Prinsen (1996)
TNO-04 (Detergent-1 ³)	n.p.	undiluted	2B	2A	III	III	NI	NI	Prinsen (1996)
TNO-05 (Silicone powder-1)	n.p.	undiluted	NI	NI	IV	IV	NI	NI	Prinsen (1996)
TNO-06 (Lubricant)	n.p.	undiluted	NI	NI	IV	IV	NI	NI	Prinsen (1996)
TNO-07 (Ink-1)	n.p.	undiluted	NI	NI	IV	IV	NI	NI	Prinsen (1996)
TNO-08 (Ink-2)	n.p.	undiluted	NI	NI	IV	IV	NI	NI	Prinsen (1996)
TNO-09 (Paint)	n.p.	undiluted	NI	NI	IV	II	NI	NI	Prinsen (1996)
TNO-10 (Silicone powder-2)	n.p.	undiluted	NI	NI	IV	IV	NI	NI	Prinsen (1996)

In Vivo and In Vitro Data Comparison
Sorted by Substance

Substance/Product Name	CASRN	Concentration Tested	In Vitro Classification (GHS)	In Vivo Classification (GHS)	In Vitro Classification (EPA)	In Vivo Classification (EPA)	In Vitro Classification (EU)	In Vivo Classification (EU)	Reference
TNO-11 (Sodium p-styrene sulfonate)	2695-37-6	undiluted	2A	SCNM	II	SCNM	R36	SCNM	Prinsen (1996)
TNO-12 (Formulation-3)	n.p.	undiluted	2A	NI	II	SCNM	R36	R36	Prinsen (1996)
TNO-13 (Pesticide-2)	n.p.	undiluted	NI	NI	IV	IV	NI	NI	Prinsen (1996)
TNO-14 (Polydisaccharide)	n.p.	14.5%	NI	NI	IV	IV	NI	NI	Prinsen (1996)
TNO-15 (Polydisaccharide)	n.p.	50%	NI	NI	IV	IV	NI	NI	Prinsen (1996)
TNO-16 (Liquid nylon product)	n.p.	undiluted	NI	NI	IV	IV	NI	NI	Prinsen (1996)
TNO-17 (Solvent-1)	n.p.	undiluted	NI	NI	IV	IV	NI	NI	Prinsen (1996)
TNO-18 (Solvent-2)	n.p.	undiluted	NI	NI	IV	IV	NI	NI	Prinsen (1996)
TNO-19 (Solvent-3)	n.p.	undiluted	NI	NI	IV	IV	NI	NI	Prinsen (1996)
TNO-20 (Solvent-4)	n.p.	undiluted	NI	NI	IV	IV	NI	NI	Prinsen (1996)
TNO-21 (Solvent-5)	n.p.	undiluted	NI	NI	IV	IV	NI	NI	Prinsen (1996)
TNO-22 (Solvent-6)	n.p.	undiluted	NI	NI	IV	IV	NI	NI	Prinsen (1996)
TNO-23 (Solvent-7)	n.p.	undiluted	NI	NI	IV	IV	NI	NI	Prinsen (1996)
TNO-24 (Solvent-8)	n.p.	undiluted	NI	NI	IV	IV	NI	NI	Prinsen (1996)
TNO-25 (Solvent-9)	n.p.	undiluted	NI	NI	IV	IV	NI	NI	Prinsen (1996)
TNO-26 (Ink-3)	n.p.	undiluted	NI	NI	IV	IV	NI	NI	Prinsen (1996)
TNO-27 (Thermal paper coating-1)	n.p.	undiluted	2B	2B	III	III	NI	NI	Prinsen (1996)
TNO-28 (Toilet cleaner-1)	n.p.	undiluted	2B	I	III	I	NI	R41	Prinsen (1996)
TNO-29 (Toilet cleaner-2)	n.p.	undiluted	2B	2A	III	III	NI	R36	Prinsen (1996)
TNO-30 (Pesticide-3)	n.p.	undiluted	2B	NI	III	IV	NI	NI	Prinsen (1996)
TNO-31 (Sulfur)	7704-34-9	undiluted	NI	NI	IV	III	NI	NI	Prinsen (1996)
TNO-32 (Ink-4)	n.p.	undiluted	2B	NI	III	IV	NI	NI	Prinsen (1996)
TNO-33 (Thermal paper coating-2)	n.p.	undiluted	2B	NI	III	IV	NI	NI	Prinsen (1996)
TNO-34 (Detergent-2)	n.p.	undiluted	I	SCNM	I	SCNM	R41	SCNM	Prinsen (1996)
TNO-35 (Propyl-lactate)	616-09-1	undiluted	I	I	I	I	R41	R41	Prinsen (1996)
TNO-36 (Ethylhexyl lactate)	6283-86-9	undiluted	2A	SCNM	II	II	R36	SCNM	Prinsen (1996)
TNO-37 (Pesticide-4)	n.p.	undiluted	2B	2B	III	III	NI	NI	Prinsen (1996)
TNO-38 (Solvent-10)	n.p.	undiluted	NI	NI	IV	IV	NI	NI	Prinsen (1996)
TNO-39 (Detergent-3)	n.p.	undiluted	NI	NI	IV	IV	NI	NI	Prinsen (1996)
TNO-40 (Glycolbromoacetate form.)	n.p.	undiluted	I	-	I	-	R41	R41 (SC)	Prinsen (1996)
TNO-41 (Amidosulfonic acid)	5329-14-6	undiluted	I	-	I	-	R41	R41 (SC)	Prinsen (1996)
TNO-42 (Glycolbromoacetate)	3785-34-0	85%	I	-	I	-	R41	R41 (SC)	Prinsen (1996)
TNO-43 (Monobromoacetic acid)	79-08-3	undiluted	I	-	I	-	R41	R41 (SC)	Prinsen (1996)
TNO-44 (Didecyldimethylammoniumchloride (23% in propyl glycol))	7173-51-5	23%	I	-	I	-	R41	R41 (SC)	Prinsen (1996)
TNO-45	n.p.	undiluted	NI	NI	NI	IV	NI	NI	Prinsen (2005)
TNO-46	n.p.	undiluted	NI	NI	NI	IV	NI	NI	Prinsen (2005)
TNO-47	n.p.	undiluted	NI	NI	NI	IV	NI	NI	Prinsen (2005)
TNO-48	n.p.	undiluted	2A	-	II	-	R36	R41 (SC)	Prinsen (2005)
TNO-49	n.p.	undiluted	I	-	I	-	R41	R41 (SC)	Prinsen (2005)
TNO-50	n.p.	undiluted	I	-	I	-	R41	R41 (SC)	Prinsen (2005)
TNO-51	n.p.	undiluted	I	-	I	-	R41	R41 (SC)	Prinsen (2005)
TNO-52	n.p.	undiluted	2B	2A	III	III	NI	R36	Prinsen (2005)
TNO-53	n.p.	undiluted	NI	NI	NI	IV	NI	NI	Prinsen (2005)

**In Vivo and In Vitro Data Comparison
Sorted by Substance**

Substance/Product Name	CASRN	Concentration Tested	In Vitro Classification (GHS)	In Vivo Classification (GHS)	In Vitro Classification (EPA)	In Vivo Classification (EPA)	In Vitro Classification (EU)	In Vivo Classification (EU)	Reference
TNO-54	n.p.	undiluted	2B	2B	III	III	NI	NI	Prinsen (2005)
TNO-55	n.p.	undiluted	2B	2A	III	III	R36	R36	Prinsen (2005)
TNO-56	n.p.	undiluted	2B	2B	III	III	R36	NI	Prinsen (2005)
TNO-57	n.p.	undiluted	2B	NI	III	IV	NI	NI	Prinsen (2005)
TNO-58	n.p.	undiluted	NI	NI	NI	IV	NI	NI	Prinsen (2005)
TNO-59	n.p.	undiluted	NI	NI	NI	IV	NI	NI	Prinsen (2005)
TNO-60	n.p.	undiluted	NI	NI	NI	IV	NI	NI	Prinsen (2005)
TNO-61	n.p.	undiluted	NI	NI	NI	IV	NI	NI	Prinsen (2005)
TNO-62	n.p.	undiluted	2B	NI	III	III	R36	NI	Prinsen (2005)
TNO-63	n.p.	undiluted	NI	NI	IV	III	NI	NI	Prinsen (2005)
TNO-64	n.p.	undiluted	2B	NI	III	IV	NI	NI	Prinsen (2005)
TNO-65	n.p.	undiluted	NI	NI	NI	IV	NI	NI	Prinsen (2005)
TNO-66	n.p.	undiluted	NI	NI	NI	IV	NI	NI	Prinsen (2005)
TNO-67	n.p.	undiluted	2B	NI	III	IV	NI	NI	Prinsen (2005)
TNO-68	n.p.	undiluted	2A	2A	II	II	R36	R36	Prinsen (2005)
TNO-69	n.p.	50%	NI	NI	NI	IV	NI	NI	Prinsen (2005)
TNO-70	n.p.	undiluted	2A	2A	II	III	R36	R36	Prinsen (2005)
TNO-71	n.p.	undiluted	2B	NI	III	IV	NI	NI	Prinsen (2005)
TNO-72	n.p.	undiluted	NI	NI	NI	IV	NI	NI	Prinsen (2005)
TNO-73	n.p.	undiluted	I	2A	I	II	R41	R36	Prinsen (2005)
TNO-74	n.p.	undiluted	NI	NI	IV	III	NI	NI	Prinsen (2005)
TNO-75	n.p.	undiluted	NI	NI	NI	IV	NI	NI	Prinsen (2005)
TNO-76	n.p.	undiluted	NI	NI	NI	IV	NI	NI	Prinsen (2005)
TNO-77	n.p.	undiluted	2B	NI	III	IV	NI	NI	Prinsen (2005)
TNO-78	n.p.	undiluted	2B	2B	III	III	NI	NI	Prinsen (2005)
TNO-79	n.p.	undiluted	2B	NI	III	IV	NI	NI	Prinsen (2005)
TNO-80	n.p.	undiluted	NI	NI	NI	IV	NI	NI	Prinsen (2005)
TNO-81	n.p.	undiluted	NI	NI	NI	IV	NI	NI	Prinsen (2005)
TNO-82	n.p.	undiluted	NI	NI	NI	IV	NI	NI	Prinsen (2005)
TNO-83	n.p.	undiluted	2B	2B	III	III	NI	R36	Prinsen (2005)
TNO-84	n.p.	undiluted	2B	NI	III	IV	NI	NI	Prinsen (2005)
TNO-85	n.p.	undiluted	2B	I	III	I	R36	R41	Prinsen (2005)
TNO-86	n.p.	undiluted	2B	NI	III	IV	NI	NI	Prinsen (2005)
TNO-87	n.p.	undiluted	2B	NI	III	IV	NI	NI	Prinsen (2005)
TNO-88	n.p.	undiluted	NI	NI	NI	IV	NI	NI	Prinsen (2005)
TNO-89	n.p.	undiluted	NI	NI	NI	IV	NI	NI	Prinsen (2005)
TNO-90	n.p.	undiluted	NI	NI	NI	IV	NI	NI	Prinsen (2005)
TNO-91	n.p.	undiluted	NI	NI	NI	IV	NI	NI	Prinsen (2005)
TNO-92	n.p.	undiluted	2B	I	III	I	R36	R41	Prinsen (2005)
TNO-93	n.p.	undiluted	2A	I	II	I	R36	R41	Prinsen (2005)
TNO-94	n.p.	undiluted	NI	I	NI	I	NI	R41	Prinsen (2005)
Toluene	108-88-3	undiluted	2A	NI	II	III	R36	NI	Balls et al. (1995)
Triacetin	102-76-1	undiluted	NI	NI	IV	IV	NI	NI	Prinsen and Koëter (1993)

**In Vivo and In Vitro Data Comparison
Sorted by Substance**

Substance/Product Name	CASRN	Concentration Tested	<i>In Vitro</i> Classification (GHS)	<i>In Vivo</i> Classification (GHS)	<i>In Vitro</i> Classification (EPA)	<i>In Vivo</i> Classification (EPA)	<i>In Vitro</i> Classification (EU)	<i>In Vivo</i> Classification (EU)	Reference
Tributyltin chloride	1461-22-9	undiluted	1	-	I	-	R41	R41	Prinsen and Koëter (1993)
Trichloroacetic acid (3%)	76-03-9	3%	2A	NI	II	III	R36	NI	Balls et al. (1995)
Trichloroacetic acid (30%)	76-03-9	30%	1	1	I	I	R41	R41	Balls et al. (1995)
Triethanolamine	102-71-6	undiluted	2B	NI	III	III	NI	NI	Prinsen and Koëter (1993)
Triton X-100 (5%)	9002-93-1	5%	2A	2A	II	III	R36	NI	Balls et al. (1995)
Triton X-100 (10%)	9002-93-1	10%	2A/2B	1	II/III	II	R36	R41	Balls et al. (1995)
Triton X-500 (5%)	—	undiluted	2B	-	III	-	NI	R36	Prinsen (2000)
Tween 20	9005-64-5	undiluted	2B	NI	III	III	NI	NI	Balls et al. (1995)

SCNM - Study criteria not met

SC - Classification assigned on the basis of skin corrosion assay