

**1,2,3, -TRINITROGLYCERIN (TNG)**  
**CAS RN: 55-63-0**  
**SUMMARY OF SIDS RESULTS**

<u>SIDS SEGMENT / TEST</u>		<u>SPECIES</u>	<u>PROTOCOL</u>	<u>RESULTS</u>
<b>PHYSICAL-CHEMICAL</b>				
1	Melting Point (°C)	--	--	2.3 ; 13.0
2	Boiling Point (°C)	--	--	Inert atmosphere: ~ 243 ± 6 (calc'd) Air: Decomposes 70
3	Vapor Pressure (kPa)	--	--	20°C = 3.6 x 10 <sup>-5</sup> ; 40°C = 3.3 x 10 <sup>-4</sup> ; 60°C = 2.3 x 10 <sup>-3</sup> (Regression line)
4	Partition Coefficient	--	--	Log P <sub>ow</sub> = 2.04
5	Water Solubility (g/L)	--	--	20°C = 1.38 – 2.0; 40°C = 1.68 60°C = 2.36; 80°C = 3.44
<b>ENVIRONMENTAL</b>				
6	Photodegradation t <sub>1/2</sub> ; (12-hr. days)	--	Footnote 1	9.741
7	Water Stability (t <sub>1/2</sub> , days)	--	--	pH 9 @ 25°C = 37; pH 5 @ 25°C = 8575 <sup>2</sup> ; pH3 @ 37°C = ">3650" .
8	Fugacity	--	EQC software	Predominantly water & soil <sup>3</sup> .
9	Biodegradation	Indigenous microorganisms downriver from plant	Footnote 1	1 <sup>st</sup> Order rate const 0.6/hr. – 8.6 x 10 <sup>-2</sup> /hr 2 <sup>nd</sup> Order constant 1.06 – 1.43 x 10 <sup>-9</sup> ml/cell/hr
9	Biodegradation	Sewage microorganisms	Footnote 1	90-100 % metabolism to DNG & MNG
<b>ECOTOXICOLOGY</b>				
10	96 hr. LC <sub>50</sub>	Rainbow trout	ASTM E729-80	1.90 mg / L
10	"	F'head Minnow	"	3.58 mg / L
10A	8 day dietary LD <sub>50</sub>	Quail <i>c. virginianus</i>	Same as OECD No. 205	>5620 ppm; LOAEL = 5620 ppm; NOAEL = 3160 ppm.
11	96 hr. EC <sub>50</sub>	Alga <i>S.capricornutum</i>	EPA 797.1060	1.15 mg / L
12	48 hr. LC <sub>50</sub>	Daph. <i>C. dubia</i>	ASTM E729-80	17.83 mg / L
<b>HEALTH</b>				
13	Acute oral LD <sub>50</sub>	Mouse	Footnote 1	M: 1,188 mg / kg (95% C.L.= 1008-1352). F: 1055 mg / kg (95% C.L. = 895 - 1178)
13	Acute oral LD <sub>50</sub>	Rat	16 CFR 1500.3 (c)(2)(I) [FHSA]	685 (95% CL=510 – 940) mg / kg
13	I.V. MLD	Rabbit	Footnote 1	45 mg / kg
13	Dermal LD <sub>50</sub>	Rat	Footnote 1	>9,560 mg / kg
13	Inhalation LC <sub>50</sub>	--	--	Not performed. Too dangerous
13	Skin irritation	Rabbit	16CFR1500.41 (FHSA)	Primary Irritation Index = 0.90
13	Eye irritation	Rabbit	16CFR 1500.42 (FHSA)	Very mild conjunctival irritation
13	Skin sensitization	Guinea pig	Kligman Maximization	4 / 10 sensitized
13A	Skin sensitization	Humans	Clinical study	Of ~6200 cases occupat'l dermatitis seen at Finnish gov't. OSH clinic, only 4 were confirmed due to TNG

<b>GENETIC TOXICITY <i>IN VIVO</i></b>				
	Dominant Lethal (diet)	Rat	~Same as OECD #478	No effect at maximum test level. (1.0 % in diet for 13 weeks)
14	Chromosome aberrations (diet)	M & F Rats (kidney cells)	~Same as OECD #475	No apparent effect @ ~230 mg/kg for eight weeks.
14	Chromosome aberrations (diet)	M & F Rats (lymphocytes)	~Same as OECD #475	No apparent effect @ ~230 mg/kg for eight weeks.
14	Chromosome aberrations (diet)	M & F Rats (bone marrow)	~Same as OECD #475	No apparent effect @ 360 mg/kg (M) or 430 mg/kg (F) for 2 years.
14	Chromosome aberrations (diet)	M & F Rats (kidney cells)	~Same as OECD #475	No apparent effect @ 360 mg/kg (M) or 430 mg/kg (F) for 2 years.
14	Chromosome aberrations (oral capsule)	M & F Dogs (kidney cells)	~Same as OECD #475	No apparent effect @ 5 mg/kg for eight weeks.
14	Chromosome aberrations (oral capsule)	M & F Dogs (lymphocytes)	~Same as OECD #475	No apparent effect @ 5 mg/kg for eight weeks.
<b>GENETIC TOXICITY <i>IN VITRO</i></b>				
15	CHO-K1 cells	Chinese hamster (K-1 cells)	~Same as OECD #476	No mutagenic effects.
15	Ames (TNG in DMSO; 1980)	S. typhimurium mutants	~Same as OECD #471	Active in TA 1537 @ 1mg a.i. / plate.
15	Ames (TNG in Ethanol)	S. typhimurium mutants	~Same as OECD #471	Active in TA 1535 @ 0.5 & 1.5 mg / plate .
15	Ames (TNG adsorbed on lactose. Suspended in DMSO; 1975 )	S. typhimurium mutants	~Same as OECD #471	Active in TA 1535 @ 0.75 & 1.0 mg / plate
<b>REPEATED DOSE TOXICITY</b>				
16	1 Yr. Oral Capsule	M & F Beagle dog	~Same as OECD #452	Methemoglobin formation in M & F at lowest dose (1 mg / kg).
16	2 Yr. Diet	M & F Rat	~Same as OECD #452	Increased foci of hepatocellular alteration (both sexes). Spleen hyperpigmentation Interstitial cell tumors (male testes). Kidney epithelial hyperpigment'n Multiple blood chem. changes Incr. liver neoplastic nodules and Hepatocellular carcinomas NOAEL: M = 3.04 mg TNG/kg/day F = 3.99 mg/kg TNG/day <u>TD</u> <sub>50</sub> <sup>5</sup> M, mixed liver = 221 mg/kg/day M, Testic. interst.=405 mg/kg/day F, mixed liver = 329 mg/kg/day
16	2 Yr. Diet	M & F Mouse	~Same as OECD #452	Decr. food intake & wt. gain; behavioral effects; methHb format'n. NOAEL: M = 114.6 mg / kg / day F = 96.4 mg / kg / day
17	3-Gen. Reproduction	Rat	U.S. FDA (1966)	Aspermatogenesis in F2a males <sup>4</sup> . Decr. food intake in F <sub>1b</sub> Females <sup>4</sup> . Reduced total litter wt. (F <sub>1b</sub> ) <sup>4</sup> . NOAEL: M = 39 mg/kg/day F = 46 mg / kg / day
18	Teratogenicity	Rat	U.S. FDA (1966)	Decr. b.wt., high dose. Incr. diaphrag. hernias, high dose Decr. Hyoid bone ossific, high dose

SPECIAL	Methemoglobinemia protection / antidote	M & F Beagle dog	Footnote 1	Methylene blue depresses MetHb formation; does not hasten removal.
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1. EPA's AOPWIN subprogram in their EPIWIN suite of environmental programs for computers.
2. Calculation by Robust Summary author, based on  $t_{1/2} = 134$  days @ 85°C. Assumes reaction rate halves for every 10°C drop in temperature.
3. Level III values in water and soil lower than Level II values. Amounts of decrease vary depending on effects of water pH, photolysis, and biodegradation.
4. At 1% dietary dose.
5. TD<sub>50</sub> (50% tumor dose); see Gold & Zeiger (1997).

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