

Nitroglycerine - Toxicological and Physiochemical Data

Parameter	Data in units from original source	Original Source	Calculation for use in the SNIFFER model	Value for input into the SNIFFER model
TDI oral	N/A		N/A	N/A
TDI inhalation	0.01ppm (0.09 mg/m ³)	NOAEL for exposure by workers - American Conference of Governmental Industrial Hygienists (2001),	Rosenblatt et al (1983) based on the assumption of 100% absorption. See Note 1 (TDI=(1.234*8*0.09*5)/(68.5*7*10))	0.0009 mg/kg bw/day
TDI dermal	N/A		N/A	N/A
Index Dose (ID) oral	Threshold		-	N/A
Index Dose (ID) inhalation	Threshold		-	N/A
Dietary Exposure	-	Exposure of the general population to NG is not thought to be likely. No data has been found relating to background levels of NG in the wider environment or in foodstuffs. Background intake of NG is therefore considered to be negligible.	-	ND
Exposure to drinking water	-	Exposure of the general population to NG is not thought to be likely. No data has been found relating to background levels of NG in drinking water.	-	ND
Adult MDI oral	-	See above	-	ND
Adult MDI inhalation	-	See above	-	ND
CASRN	55-63-0	Collation of Toxicological Data and Development of Guideline Values for Explosive Substances: Collation of Physiochemical Data. EA R&D Document P5-036/01	-	55-63-0
Relative molecular weight	227.11 g.mol ⁻¹		-	227.11 g.mol ⁻¹
Vapour pressure	0.196 Pa @ 20°C		Divide by 133.3 to convert Pa to mmHg	1.47E-03 mmHg
Aqueous solubility	1800 mg/l @ 20°C		-	1880 mg/L
Henry's Law Constant	1.02E-05 dimensionless			1.02E-05 dimensionless
Kow	50 dimensionless			50 dimensionless
Koc	589 (cm ³ .g ⁻¹)			589 (cm ³ .g ⁻¹)
Diffusion in air	7.0E-06 m ² .s ⁻¹			7.0E-06 m ² .s ⁻¹
Diffusion in water	6.1E-10 m ² .s ⁻¹			6.1E-10 m ² .s ⁻¹
Dermal-soil adsorption adjustment factor	0.1		US EPA 1999 "Risk Assessment Guidance for Superfund Volume I: Human Health Evaluation Manual (Part E, Supplemental Guidance for Dermal Risk Assessment) Interim Guidance"	N/A

Nitroglycerine - Toxicological and Physiochemical Data

Note:

- (1) Rosenblatt et al (1983) outline a method to convert occupational exposure data into a TDI. On the assumption of 100% absorption by the lungs and that the target organ is the same whatever the uptake route (EA, 2002a) the following conversion can be applied to both the TLV of 0.46 mg m⁻³ or the ACGIH (2001) LOEL concentration of 0.03 ppm (0.28 mg m⁻³). As occupational health limits are designed to protect workers i.e. adults, the conversion uses details given in CLR10 (EA, 2002b) for an adult female. This calculated TDI could then be applied to any age class; a safety factor of 10 is applied to the calculation to reflect the position of this data source in the adopted data hierarchy and the assumptions required to apply the calculation to any age class.

$$\text{TDI} = \frac{\text{Breathing rate (active female m}^3 \text{ h}^{-1}) \times 8\text{hrs} \times \text{exposure conc. (mg m}^{-3}) \times 5 \text{ working days}}{\text{Bodyweight (kg)} \times 7 \text{ day week} \times \text{safety factor}}$$