TC NES SUBGROUP ON IDENTIFICATION OF PBT AND VPVB SUBSTANCES

RESULTS OF THE EVALUATION OF THE PBT/VPVB PROPERTIES OF:

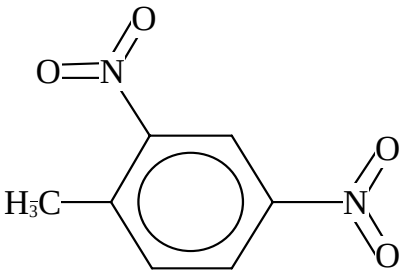
Substance name: 2,4-dinitrotoluene

EC number: 204-450-0

CAS number: 121-14-2

Molecular formula: C7H6N2O4

Structural formula:



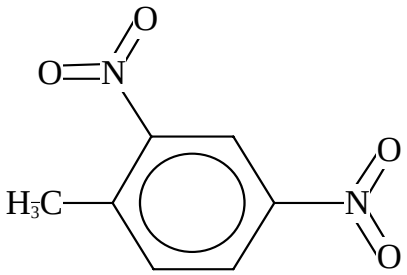
Summary of the evaluation:

2,4-dinitrotoluene is not considered to be a PBT substance. It does not meet the B criterion. The T criterion is not met for ecotoxicity but for effects on human health. The substance may meet the P/vP criteria based on screening data.

JUSTIFICATION

1 IDENTIFICATION OF THE SUBSTANCE AND PHYSICAL AND CHEMICAL PROPERTIES

Name: 2,4-dinitrotoluene
EC Number: 204-450-0
CAS Number: 121-14-2
IUPAC Name: Benzene,1-methyl-2,4-dinitro
Molecular Formula: C7H6N2O4
Structural Formula:



Molecular Weight: 182.13
Synonyms: Dinitrotoluene, technical grade; 1,3-Dinitro-4-methylbenzene; 1-Methyl-2,4-dinitrobenzene; 2,4-Dinitro-1-methylbenzene; 2,4-DNT (abbreviation)

1.1 PURITY/IMPURITIES/ADDITIVES

No data available.

1.2 PHYSICO-CHEMICAL PROPERTIES

Table 1 Summary of physico-chemical properties. For details and references, see GDCh (1987) and European Commission (2005)

REACH ref Annex, §	Property	Value	Comments
V, 5.1	Physical state at 20 C and 101.3 Kpa	solid	
V, 5.2	Melting/freezing point	69.9ºC	Bayer AG
V, 5.3	Boiling point	319.5ºC	Bayer AG
V, 5.5	Vapour pressure	7.9 10^{-3} Pa at 20ºC	Bayer AG
V, 5.7	Water solubility	166 mg l^{-1} at room temperature 446.2 mg l^{-1} at 25ºC 270 mg l^{-1} at 22ºC	Bayer AG Calculated (WSKOW v1.41) WSKOW exper. database (Spanggord et al., 1980) (data not evaluated)
V, 5.8	Partition coefficient n-octanol/ water (log value)	2.18 1.98	Calculated (KOWWIN v 1.67) KOWWIN exper. database (Hansch et al., 1995) (data not evaluated)
VII, 5.19	Dissociation constant		

2 MANUFACTURE AND USES

The substance is used as an intermediate. The production/import volume of companies which provided information under Regulation 93/793/EEC is 100,000 – 500,000 tonnes/year.

3 CLASSIFICATION AND LABELLING

The substance is included in the Annex I of Directive 67/548/EEC with the following classification:

Carc. Cat 2, R45	May cause cancer
Muta. Cat. 3; R68	Possible risk of irreversible effects
Repr. Cat. 3; R62	Possible risk of impaired fertility
T; R23/24/25	Toxic by inhalation, in contact with skin and if swallowed
Xn; R48/22	Harmful: danger of serious damage to health by prolonged exposure if swallowed
N; R51-53	Toxic to aquatic organisms, may cause long-term adverse effects in the aquatic environment

4 ENVIRONMENTAL FATE PROPERTIES

4.1 DEGRADATION (P)

4.1.1 Abiotic degradation

Indirect photochemical degradation in the atmosphere is considered to be very slow based on the estimated half-life of 74 days for the reaction with OH-radicals using AOP v1.91 (24 h day^{-1}; $5 \cdot 10^5$ OH^- cm^{-3}).

Data on abiotic degradation have been reviewed by European Commission (2005).

4.1.2 Biotic degradation

A ready biodegradability test (similar to OECD 301D) using isomer mixture (80% 2,4-DNT: 20% 2,6-DNT) resulted 0% degradation in 28 days (MITI, 1992). A screening test using anaerobic conditions and similar isomer mixture showed no degradation in 56 days (Bayer AG, 1991). 2,4-dinitrotoluene seems to degrade in biodegradation tests using adapted inocula and certain microbial strains or in tests employing very favourable conditions for biodegradation. The available results have been reviewed in the EU risk assessment of 2,4-DNT (European Commission, 2005) and in the SIAR of the isomer mixture (OECD, 2004).

4.1.3 Other information [1]

Data not reviewed for this report.

4.1.4 Summary and discussion of persistence

The results of the available biodegradation screening tests indicate that the substance is not readily biodegradable but inherently degradable when using adapted micro-organisms. Simulation tests would be needed to determine biodegradation half-lives relevant for the environmental conditions. For the EU risk assessment, following half-lives were used for the exposure estimation (European Commission, 2005).

Compartment		Half-life
Atmospheric		71 days
Aquatic	Abiotic degradation	48 days
	Biodegradation	∞ days
Sediment		3,014 days
Soil		300 days

[1] For example, half life from field studies or monitoring data

4.2 ENVIRONMENTAL DISTRIBUTION

The available data are reviewed by European Commission (2005).

4.2.1 Adsorption

4.2.2 Volatilisation

4.2.3 Long-range environmental transport

Based on the estimated atmospheric half-life, 2,4-DNT has a very high potential for long-range atmospheric transport, if emitted to air.

4.3 BIOACCUMULATION (B)

4.3.1 Screening data[2]

The derived octanol-water partitioning coefficients (logKow) are around 2. An estimated BCF of 6.7 was derived by BCFWIN v2.15 using logKow of 1.98. The European Commission (2005) reports a calculated BCF of 7.65 for fish using the method of the TGD.

4.3.2 Measured bioaccumulation data[3]

Daphnia magna was tested with ^{14}C-labelled 2,4-dinitrotoluene four days in a concentration of 1 mg l^{-1}. A whole body BCF of 13 was determined (Liu et al., 1983). For *Lumbriculus variegatus* a BCF of 58, for *Lepomis macrochirus* a BCF between 4 and 78 (muscle and viscera measured separately) and for *Selenastrum capricornutum* a BCF of 2507 were determined in a similar test procedure (Liu et al., 1983). *L. macrochirus* was depurated after the uptake phase and it was concluded that uptake of 2,4-DNT was low and elimination fast and that nearly all of the substance taken up was depurated within three days. The BCF observed for algae cannot be used for the evaluation of the bioaccumulation potential as adsorption may have influenced the results.

Additional bioaccumulation results are described in detail in the EU risk assessment of 2,4-DNT (European Commission, 2005) and they support the findings described above.

4.3.3 Other supporting information[4]

4.3.4 Summary and discussion of bioaccumulation

The experimental bioconcentration factors and the available logKow –values indicate low to moderate bioaccumulation potential.

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2 For example, log K_{ow} values, predicted BCFs

3 For example, fish bioconcentration factor

4For example, measured concentrations in biota

5 HUMAN HEALTH HAZARD ASSESSMENT

Data not reviewed for this report.

6 ENVIRONMENTAL HAZARD ASSESSMENT

6.1 AQUATIC COMPARTMENT (INCLUDING SEDIMENT)

6.1.1 Toxicity test results

6.1.1.1 Fish

Acute toxicity

Long-term toxicity

Five fish species have been tested for long-term effects. Reliable NOECs in the range of 0.28-3.4 mg l^{-1} have been observed.

6.1.1.2 Aquatic invertebrates

Acute toxicity

Long-term toxicity

A 21-day reproduction study of Kühn et al (1988) with *D. magna* gave a NOEC of 0.04 mg l^{-1}. The method applied is "Proposed Preliminary Testing method: Prolonged toxicity Test on *Daphnia magna"* (Federal Environment Agency, Germany, 1984). As the limit of detection was 0.05 mg l^{-1}, the NOEC was determined using the recovery rate of the measured concentrations (note: the EU risk assessment uses a 50% recovery resulting a NOEC of 0.02 mg l^{-1}). Two other studies on *Daphnia magna* gave NOECs in the same order of magnitude.

6.1.1.3 Algae and aquatic plants

Algae toxicity results are available for green algae, diatoms and blue-green algae. NOECs (or EC_{10}) in the range of 0.13-1.9 mg l^{-1} have been found.

6.1.2 Sediment organisms

Data not reviewed for this report.

6.1.3 Other aquatic organisms

Data not reviewed for this report.

6.2 TERRESTRIAL COMPARTMENT

Data not reviewed for this report.

6.3 ATMOSPHERIC COMPARTMENT

Data not reviewed for this report.

7 PBT AND VPVB

7.1 PBT, VPVB ASSESSMENT

Persistence: 2,4-dinitrotoluene (2,4-DNT) is considered to meet the P/vP screening criterion. The available screening tests indicate that the substance is not readily biodegradable, but it is inherently degradable when using adapted micro-organisms. Degradation simulation testing would be necessary to assess the biodegradation rate in the environmentally relevant conditions. However, there is no need for further information in the frame of the PBT assessment (see below).

Bioaccumulation: 2,4-DNT does not meet the B criterion. The low octanol-water partitioning coefficient (logKow is approximately 2) and the experimental bioconcentration factors (BCFs up to 78) indicate low to moderate bioaccumulation potential.

Toxicity: Data on long-term effects are available for fish, daphnids and algae. The lowest long-term (21 d) NOEC has been determined as 0.02 mg $l^{-1}$with *Daphnia magna*, and so the substance does not meet the T criterion for ecotoxicity. Nevertheless, T criterion is considered fulfilled due to the human health hazard classification (Carcinogenic cat 2, Toxic for Reproduction, cat 3).

Summary: 2,4-dinitrotoluene may meet the P/vP criterion based on screening data and it is considered to meet the T criterion for human health but not for ecotoxicity. The substance does not meet the B criterion, and therefore it is not considered as a PBT substance.

INFORMATION ON USE AND EXPOSURE

Not relevant as the substance is not identified as a PBT.

OTHER INFORMATION

The information and references used in this report were taken from the following sources:

European Commission (2005) European Union Risk Assessment Report, Draft of November 2005, 2,4-dinitrotoluene, CAS No: 121-14-2, EINECS No: 204-450-0.

GDCh (1987) BUA-Stoffbericht: Nr. 12. Dinitrotoluol. Edited by GDCh-Advisory Committee on Existing Chemicals of Environmental Relevance (BUA). VCH Verlagsgesellschaft, Weinheim.

OECD (2004) Dinitrotoluene (isomers mixture), CAS 25321-14-6. SIDS Initial Assessment Report for SIAM 18, Paris, France, April 20-23, 2004.