GHS Classification

ID414 2,6-Dinitrotoluene

CAS 606-20-2 Date Classified: Aug. 22, 2006 (Environmental Hazards: Mar. 31, 2006)

Physical Hazards Reference Manual: GHS Classification Manual (Feb. 10, 2006)

Hazard class		Classification	symbol	signal word	hazard statement	Rational for the classification
1	Explosives	Not classified	–	–	–	Because of a lack of data on the kick-off temperature and decomposition energy (though the substance contains nitro groups with its oxygen budget calculated at -114, and may explode if heated according to ICSC (2004)). Classified as Division 6.1 (UN#3454 (solid) and UN#1600 (molten)) (UN Recommendations on the Transport of Dangerous Goods). Commercial 2,4-dinitrotoluene, which contains about 20% of 2,6-dinitrotoluene, starts to decompose at 250degC -- a process that continues at 280degC (Bretherick (J), 5th, 1998). The decomposition energy stands at about 85% of that of TNT (2,4,6-trinitrotoluene) (5.1kJ/g) (Bretherick (J), 5th, 1998), according to some reports (NFPA, 13th, 2002).
2	Flammable gases	Not applicable	–	–	–	Classified as "solid" according to GHS definition
3	Flammable aerosols	Not applicable	–	–	–	Not aerosol products
4	Oxidizing gases	Not applicable	–	–	–	Classified as "solid" according to GHS definition
5	Gases under pressure	Not applicable	–	–	–	Classified as "solid" according to GHS definition
6	Flammable liquids	Not applicable	–	–	–	Classified as "solid" according to GHS definition
7	Flammable solids	Not classified	–	–	–	Classified as flammable according to ICSC (2004). Classified intoo Division 6.1 (UN#3454 (solid) and UN#1600 (molten)) (UN Recommendations on the Transport of Dangerous Goods).
8	Self-reactive substances and mixtures	Not classified	–	–	–	Containing nitro groups with explosive properties. The substance may explode if heated according to ICSC (2004)). Classified into Division 6.1 (UN#3454 (solid) and 1600 (molten)) (UN Recommendations on the Transport of Dangerous Goods).
9	Pyrophoric liquids	Not applicable	–	–	–	Classified as "solid" according to GHS definition
10	Pyrophoric solids	Not classified	–	–	–	Classified into Division 6.1 (UN#3454 (solid) and 1600 (molten)) (UN Recommendations on the Transport of Dangerous Goods).
11	Self-heating substances and mixtures	Classification not possible	–	–	–	Test methods applicable to liquid substances are not available (melting point: 66degC (ICSC, 2004), test temperature: 140degC).
12	Substances and mixtures, which in contact with water, emit flammable gases	Not applicable	–	–	–	Containing no metals or metalloids (B, Si, P, Ge, As, Se, Sn, Sb, Te, Bi, Po, At)
13	Oxidizing liquids	Not applicable	–	–	–	Classified as "solid" according to GHS definition
14	Oxidizing solids	Not classified	–	–	–	No data available, though being organic compounds containing oxygen bound to elements other than carbon and hydrogen. Classified into Division 6.1 (UN#3454 (solid) and 1600 (molten)) (UN Recommendations on the Transport of Dangerous Goods).
15	Organic peroxides	Not applicable	–	–	–	Organic compounds containing no "-O-O-" structure
16	Corrosive to metals	Classification not possible	–	–	–	Test methods applicable to solid substances are not available

Health Hazards

Hazard class		Classification	symbol	signal word	hazard statement	Rational for the classification
1	Acute toxicity (oral)	Category 3	Skull and crossbones	Danger	Toxic if swallowed	Based on the LD50 value of 177mg/kg calculated from the testing data of rat LD50 (oral route) of 177mg/kg (MOE Risk Assessment vol. 4 (2005)), 180mg/kg (IARC (1996)), 535mg/kg (SIDS (2005)) and 795mg/kg (CERI Hazard Data 98-15(3) (1998)).
1	Acute toxicity (dermal)	Classification not possible	–	–	–	No data available
1	Acute toxicity (inhalation: gas)	Not applicable	–	–	–	Due to the fact that the substance is "solid" according to the GHS definition and inhalation of its gas is not expected.
1	Acute toxicity (inhalation:	Classification not possible	–	–	–	No data available
1	Acute toxicity (inhalation: dust, mist)	Not classified	–	–	–	Based on the rat LC50 (4 hour inhalation) value of 360mg/L (CERI Hazard Data 98-15(3) (1998)).
2	Skin corrosion / irritation	Not classified	–	–	–	Based on the results of rabbit skin irritation tests that suggest no skin irritation (CERI Hazard Data 98-15(3) (1998)).
3	Serious eye damage / eye irritation	Not classified	–	–	–	Based on the results of rabbit eye irritation tests that suggest no eye irritation (CERI Hazard Data 98-15(3) (1998)).
4	Respiratory/skin sensitization	Respiratory sensitization: Classification not possible Skin sensitization: Classification not possible	(Respiratory sensitization)- (Skin sensitization)-	(Respiratory sensitization)- (Skin sensitization)-	(Respiratory sensitization)- (Skin sensitization)-	Respiratory sensitization: No data available Skin sensitization: Insufficient data available
5	Germ cell mutagenicity	Category 2	Health hazard	Warning	Suspected of causing genetic defects	Based on the absence of data on multi-generation mutagenicity tests and germ/somatic cell mutagenicity tests in vivo, and positive data on somatic cell genotoxicity tests in vivo (unscheduled DNA synthesis tests, DNA bonding tests) and mutagenicity tests in vitro (reverse mutation tests), described in CERI-NITE Hazard Assessment No.51 (2004), NITE Initial Risk Assessment No.51 (2005), CERI Hazard Data 98-15(2) (1999), NTP DB (Access on April 2006), ATSDR (1998), IARC 9 (1975) and DFGOT vol.6 (1994).
6	Carcinogenicity	Category 2	Health hazard	Warning	Suspected of causing cancer	Due to the fact that the substance is classified as Group 2B by IARC (1999), Category B2 by EPA (1990) and Category 2B by the Japan Society for Occupational Health.
7	Toxic to reproduction	Category 2	Health hazard	Warning	Suspected of damaging fertility or the unborn child	Based on the evidence of atrophy of the testes along with a reduction in the level of (or lack of) sperm production found in reproductive toxicity studies in mice, described in MOE Risk Assessment vol. 4 (2005) (though no data are available on general toxicity).

8	Specific target organs/systemic toxicity following single exposure	Category 1 (liver, nervous system, respiratory organs), Category 2 (cardiovascular system, blood system), Category 3 (narcotic effects)	Health hazard	Danger	Causes damage to organs (liver, nervous system, respiratory organs) May cause damage to organs (cardiovascular system, blood system) (Narcotic effects) May cause drowsiness or dizziness	Based on the human evidence: "adversely affects the central nervous system, cardiovascular system and blood, and may produce methemoglobin" (ICSC (J) (1997)). Also based on the evidence from animal studies including "widespread centrolobular hepatocyte hemorrhagic necrosis and some deaths" (CERI-NITE Hazard Assessment No.51 (2004)), "died after developing respiratory depression, ataxia and lethargy" (SIDS (2004)). The effects on experimental animals were observed at dosing levels within the guidance value ranges for Category 1. Since the priority rating of the studies on human health effects is 2, the effects on the cardiovascular system and blood system are classified into Category 2. Refer to "Dinitrotoluene (ID_0413, CAS_25321-14-6)."
9	Specific target organs/systemic toxicity following repeated exposure	Category 1 (blood system, liver) Category 2 (testes, nervous system, kidneys, cardiovascular system)	Health hazard	Danger	Causes damage to organs through prolonged or repeated exposure (blood system, liver) May cause damage to organs through prolonged or repeated exposure (testes, nervous system, kidneys, cardiovascular system)	Based on the human evidence: "adversely affects the central nervous system, cardiovascular system and blood, and may produce methemoglobin" (ICSC (J) (1997)). Also based on the evidence from animal studies "increased extramedullary hematopoiesis in the spleen, testicular atrophy, reduced sperm productivity, hyperplasia of bile-duct epithelium," "paralysis associated with tetany and spasm, anemia, methemoglobinemia, increased platelet, decreased lymphocytes, increased alkaline phosphatase, increased ALT/urea nitrogen, increased extramedullary hematopoiesis in the spleen, hyperplasia of bile-duct epithelium, hepatic degeneration/inflammation, renal degeneration/inflammation, and testicular atrophy were observed" (CERI-NITE Hazard Assessment No.51 (2004)), "hyperplasia of bile-duct epithelium, hepatocyte degeneration and vacuolization were found" (MOE Risk Assessment vol. 4 (2005)). The effects on experimental animals were observed at dosing levels within the guidance value ranges for Category 1 (blood system, liver) and Category 2 (testes, nervous system, kidneys). The effects on the cardiovascular system is classified into Category 2 since the priority rating of the referenced study is 2. Refer to "Dinitrotoluene (ID_0413, CAS_25321-14-6)."
10	Aspiration hazard	Classification not possible	—	—	—	No data available

Environmental Hazards

Hazard class		Classification	symbol	signal word	hazard statement	Rational for the classification
11	Hazardous to the aquatic environment (acute)	Category 3	-	-	Harmful to aquatic life	It was classified into Category 3 from 72 hours ErC50=15mg/L of the algae (Selenastrum) (MOE Eco-Toxicity Tests of Chemicals, 1997).
11	Hazardous to the aquatic environment (chronic)	Category 3	-	-	Harmful to aquatic life with long lasting effects	Although acute toxicity was Category 3 and the bio-accumulation potential was low (log Kow=2.1(PHYSPROP Database, 2005)), since there was no rapidly degrading (the decomposition by BOD: 0%(CERI/NITE Hazard Assessment Report, 2004)), it was classified into Category 3.