Fire Extinguishing Agents NOT to Be Used: Water
Special Hazards of Combustion Products: Not pertinent
Behavior in Fire: Containers may explode. Vapor is heavier than air and may travel a long distance to a source of ignition and flash back.
Ignition Temperature: 842° F
Electrical Hazard: Class I, Group D
Burning Rate: 8.2 mm/min.
Adiabatic Flame Temperature: 2419. (Est.)
Stoichiometric Air to Fuel Ratio: 23.8 (calc.)
Flame Temperature: Currently not available
Combustion Molar Ratio (Reactant to Product): 7.0 (calc.)

5. CHEMICAL REACTIVITY

Reactivity with Water: No reaction
Reactivity with Common Materials: No reaction
Stability During Transport: Stable
Neutralizing Agents for Acids and Caustics: Not pertinent
Polymerization: Not pertinent
Inhibitor of Polymerization: Not pertinent

6. WATER POLLUTION

Aquatic Toxicity: None
Waterfowl Toxicity: None
Biological Oxygen Demand (BOD): None
Food Chain Concentration Potential: None
GESAMP Hazard Profile:
Not listed

7. SHIPPING INFORMATION

Grades of Purity: Research; instrument, or Pure: 99.35+ % Technical: 97.50 %
Storage Temperature: Ambient
Inert Atmosphere: No requirement
Venting: Safety relief
IMO Pollution Category: Currently not available
Ship Type: 2
Barge Hull Type: Currently not available

8. HAZARD CLASSIFICATIONS

49 CFR Category: Flammable gas
49 CFR Class: 2.1
49 CFR Package Group: Not pertinent.
Marine Pollutant: No
NFPA Hazard Classificaton: 1 4 0
EPA Reportable Quantity: Not listed.
EPA Pollution Category: Not listed.
RCRA Waste Number: Not listed
EPA FWPCA List: Not listed

9. PHYSICAL AND CHEMICAL PROPERTIES

Physical State at 15 Degrees C and 1 ATM: Gas
Molecular Weight: 44.09

Boiling Point at 1 ATM: −43.8° F = −42.1° C = 231.1° K

Freezing Point: −305.9° F = −187.7° C = 85.5° K
Critical Temperature: 206.0° F = 96.67° C = 369.67° K

Critical Pressure: 616.5 psia = 41.94 atm = 4.249 MN/m^2

Specific Gravity: 0.590 at −50° C (liquid)
Liquid Surface Tension (Est.): 16 dynes/cm = 0.016 N/m at -47° C

Liquid Water Interfacial Tension: (est.) 50 dynes/cm = 0.05 N/m at −50° C
Vapor (Gas) Specific Gravity: 1.5
Ratio of Specific Heats of Vapor (Gas): 1.130

Latent Heat of Vaporization: 183.2 Btu/lb = 101.8 cal/g = 4.262 X 10^5 J/kg

Heat of Combustion: −19,782 Btu/lb = −10,990 cal/g = −460.13 X 10^5 J/kg
Heat of Decomposition: Not pertinent
Heat of Solution: Not pertinent
Heat of Polymerization: Not pertinent
Heat of Fusion: Currently not available
Limiting Value: Currently not available
REID Vapor Pressure: 190 psia

UN TDG, 2007

UN No.	Name and description	Class or division	Subsidiary risk	UN packing group	Special provisions	Limited and excepted quantities		Packagings and IBCs		Portable tanks and bulk containers	
								Packing instruction	Special packing provisions	Instructions	Special provisions
(1)	(2)	(3)	(4)	(5)	(6)	(7a)	(7b)	(8)	(9)	(10)	(11)
-	3.1.2	2.0	2.0	2.0.1.3	3.3	3.4	3.5	4.1.4	4.1.4	4.2.5 / 4.3.2	4.2.5
1964	HYDROCARBON GAS MIXTURE, COMPRESSED, N.O.S.	2.1			274	0	E0	P200			
1965	HYDROCARBON GAS MIXTURE, LIQUEFIED, N.O.S.	2.1			274	0	E0	P200		T50	
1966	HYDROGEN, REFRIGERATED LIQUID	2.1				0	E0	P203		T75	TP5 TP23 TP34
1967	INSECTICIDE GAS, TOXIC, N.O.S.	2.3			274	0	E0	P200			
1968	INSECTICIDE GAS, N.O.S.	2.2			274	120 ml	E1	P200			
1969	ISOBUTANE	2.1				0	E0	P200		T50	
1970	KRYPTON, REFRIGERATED LIQUID	2.2				120 ml	E1	P203		T75	TP5
1971	METHANE, COMPRESSED or NATURAL GAS, COMPRESSED with high methane content	2.1				0	E0	P200			
1972	METHANE, REFRIGERATED LIQUID or NATURAL GAS, REFRIGERATED LIQUID with high methane content	2.1				0	E0	P203		T75	TP5
1973	CHLORODIFLUOROMETHANE AND CHLOROPENTAFLUORO-ETHANE MIXTURE with fixed boiling point, with approximately 49% chlorodifluoromethane (REFRIGERANT GAS R 502)	2.2				120 ml	E1	P200		T50	
1974	CHLORODIFLUORO-BROMOMETHANE (REFRIGERANT GAS R 12B1)	2.2				120 ml	E1	P200		T50	
1975	NITRIC OXIDE AND DINITROGEN TETROXIDE MIXTURE (NITRIC OXIDE AND NITROGEN DIOXIDE MIXTURE)	2.3	5.1 8			0	E0	P200			
1976	OCTAFLUOROCYCLOBUTANE (REFRIGERANT GAS RC 318)	2.2				120 ml	E1	P200		T50	
1977	NITROGEN, REFRIGERATED LIQUID	2.2				120 ml	E1	P203		T75	TP5
1978	PROPANE	2.1				0	E0	P200		T50	
1982	TETRAFLUOROMETHANE (REFRIGERANT GAS R 14)	2.2				120 ml	E1	P200			
1983	1-CHLORO-2,2,2-TRIFLUOROETHANE (REFRIGERANT GAS R 133a)	2.2				120 ml	E1	P200		T50	
1984	TRIFLUOROMETHANE (REFRIGERANT GAS R 23)	2.2				120 ml	E1	P200			
1986	ALCOHOLS, FLAMMABLE, TOXIC, N.O.S.	3	6.1	I	274	0	E0	P001		T14	TP2 TP13 TP27
1986	ALCOHOLS, FLAMMABLE, TOXIC, N.O.S.	3	6.1	II	274	1 L	E2	P001 IBC02		T11	TP2 TP27
1986	ALCOHOLS, FLAMMABLE, TOXIC, N.O.S.	3	6.1	III	223 274	5 L	E1	P001 IBC03		T7	TP1 TP28
1987	ALCOHOLS, N.O.S.	3		II	274	1 L	E2	P001 IBC02		T7	TP1 TP8 TP28
1987	ALCOHOLS, N.O.S.	3		III	223 274	5 L	E1	P001 IBC03 LP01		T4	TP1 TP29

Patty, 2001

資料P-11(Patty)

1000 ppm is recommended by the ACGIH. A TLV is not recommended for each simple asphyxiant. Ethane is considered an asphyxiant in Australia, Belgium, Hungary, Mexico, The Netherlands, and the United Kingdom (19, 20). The occupational exposure limit in Switzerland is 10,000 ppm (12,500 mg/m^3) TWA (19).

3.0 Propane

3.0.1 CAS Number: [74-98-6]

3.0.2 Synonyms: Dimethylmethane; *n*-propane; propane, various grades; liquefied petroleum gas; propyl hydride

3.0.3 Trade Names: NA

3.0.4 Molecular Weight: 44.09

3.0.5 Molecular Formula: $CH_3CH_2CH_3$

3.0.6 Molecular Structure:

3.1 Chemical and Physical Properties

3.1.1 General

Propane, C_3H_8, is a colorless, highly flammable gas. It is a constituent in the paraffin fraction of crude oil and natural gas (16). Its specific gravity is 1.55. Selected physical data are presented in Table 49.1.

3.1.2 Odor and Warning Properties

Propane is odorless when pure; a foul smelling odorant is often added when propane is used for fuel purposes (35, 36). The odor of propane can be detected between 1800 and 36,000 mg/m^3 (21).

3.2 Production and Use

Propane is emitted into the atmosphere from furnaces, automobile exhausts, and natural gas sources and from the combustion of polyethylene and phenolic resins. Propane is used as a component of liquid petroleum gas for commercial and industrial usage; as a feedstock in thermal cracking processes, to manufacture ethylene and propylene; as a basic material in chemical synthesis, for oxidation, alkylation, nitration and chlorination; as an aerosol propellant, to replace the chlorofluorocarbons; as a refrigerant in chemical refining and gas processing operations; as a fuel in welding and cutting operations; and as a solvent and extractant in deasphalting and degreasing of crude oils (37).

3.3 Exposure Assessment

3.3.1 Air

Propane may be determined in the air using a colorimetric assay and direct-reading devices (flame ionization meter or portable thermal conductivity gas chromatography) (26).

Propane concentrations are also determined using headspace gas chromatography methods (38, 39). A hydrocarbon fast-response gas sensor has been developed to measure propane in liquefied natural gas spills (11).

3.3.2 Background Levels: NA

3.3.3 Workplace Methods: NA

3.3.4 Community Methods: NA

3.3.5 Biomonitoring/Biomarkers

Propane has been measured in blood and expired air samples using gas chromatography (37). Propane in tissues has been determined using headspace gas chromatography techniques (40).

3.4 Toxic Effects

3.4.1 Experimental Studies

3.4.1.1 Acute Toxicity. Propane is a simple asphyxiant like methane and ethane. Guinea pigs exposed to 24,000–29,000 ppm for 5–120 min showed irregular breathing. At a concentration of 47,000–55,000 ppm tremors occurred during the first 5 min of exposure. Stupor was observed in all animals exposed for ≤ 2 h. The effect was rapidly reversible on cessation of exposure (28). In cats, 93% propane is mildly anesthetic (41). In dogs, 1% propane causes hemodynamic changes, whereas 3.3% decreases inotropism of the heart; a decrease in mean aortic pressure, stroke volume, and cardiac output; and increase in pulmonary vascular resistance (42). In primates, 10% induces some myocardial effects, whereas exposure to 20% causes aggravation of these parameters and respiratory depression (43, 44). In other studies 10% propane in the mouse and 15% in the dog produced no arrhythmia but weak cardiac sensitization (29, 45).

3.4.1.2 Chronic and Subchronic Toxicity. Subchronic inhalation studies were conducted in monkeys exposed to 750 ppm for 90 consecutive days with no toxicity observed (46). In an inhalation study in monkeys exposed to an aerosol spray deodorant containing a mixture of propane and isobutane of 65% by weight, all animals survived and showed no changes in body weight, behavior, hematology, blood chemistry, urinalysis, and electrocardiogram and pulmonary function. No organ toxicity was found (47).

3.4.1.3 Pharmacokinetics, Metabolism, and Mechanisms. In mice exposed to a liquid–gas mixture containing propane, butane, and isobutane (at 17, 31, and 52%, respectively), death occurred within 15 s of exposure. Concentrations of the compound were maximal within 1 h of death and decreased thereafter. No residues or only traces were detected by day 15 postmortem. Maximum concentrations were observed in the adipose tissue 4 days after death, and the compound was still detectable by day 15 (48).

3.4.1.4 Reproductive and Developmental. Pregnant mice were exposed on gestation day 8 for one hour to a 5–8% concentration of fuel gas. In addition to 85% methane, most natural gases contain small amounts of ethane, propane, and butane. Abnormalities of the fetal brains were found to result in brain hernia and hydrocephalus (15).

3.4.1.5 Carcinogenesis: NA

3.4.1.6 Genetic and Related Cellular Effects Studies. Propane was not mutagenic when tested using the Ames *Salmonella typhimurium* system at various vapor concentrations with and without metabolic activation (46).

3.4.1.7 Other: Neurological, Pulmonary, Skin Sensitization, etc. Propane is moderately irritating to the skin of rabbits, but not to the skin of mice (46).

3.4.2 Human Experience

3.4.2.1 General Information. Propane is an anesthetic and is nonirritating to the eyes, nose, or throat (7). Direct skin or mucous membrane contact with liquefied propane causes burns and frostbite (49). At air concentration levels below 1000 ppm, propane exerts very little physiological action (50). At very high levels, propane has CNS depressant and asphyxiating properties; its target organ is the central nervous system (36).

3.4.2.2 Clinical Cases

3.4.2.2.1 Acute Toxicity. There is one reported case of a man exposed to propane (concentration was not reported) from a leaking tank in an automobile. He exhibited colicky pains; became stupefied, disoriented, and excited; pupils of his eyes narrowed; and he exhibited marked salivation. The man recovered, but suffered from retrograde amnesia (16). Five female workers were exposed to propane when the gas escaped through improper pipe fittings. Headache, numbness, a "chilly feeling," and vomiting were reported (16).

3.4.2.2.2 Chronic and Subchronic Toxicity: NA

3.4.2.2.3 Pharmacokinetics, Metabolism, and Mechanisms. A death involving asphyxiation by propane inhalation has been reported. The presence of propane was determined in blood, brain, kidney, liver, and lung by gas chromatography. The brain of the deceased showed the highest level of propane, whereas the kidney exhibited the lowest level (40). Twenty cases of "sudden death" have been reported in which propane and propylene were quantified in blood, urine, and cerebrospinal fluid (5). Traces of propane have been measured in human expired air (51).

3.4.2.3 Epidemiology Studies

3.4.2.3.1 Acute Toxicity. Eight adult volunteers of both sexes were exposed to isobutane, propane, or mixtures of both gases (250–1000 ppm for 1, 5, and 10 min, and 1,

2 and 8 h/day for 1 day or 2 weeks) in a controlled environmental chamber for the purpose of monitoring their physiological responses. No abnormal physiological responses, cardiac abnormalities, or pulmonary function abnormalities were observed in any volunteer (52). Acute exposures of volunteers to 250, 500, or 1000 ppm for periods of 1 min to 8 h did not produce any physiological effects as determined by serial electrocardiograms or modified V5 by telemetry during exposure (53).

3.4.2.3.2 Chronic and Subchronic Toxicity: NA

3.4.2.3.3 Pharmacokinetics, Metabolism, and Mechanisms. Inhalation represents the major route by which propane is absorbed systemically. A study in human volunteers showed that blood levels of propane could be detected after exposure to 250–1000 ppm. Compared to respiratory absorption, dermal penetration of propane can be considered to be very low (52). The distribution of propane in tissues can be expected to follow the same pattern observed for butane (54).

3.4.2.3.4 Reproductive and Developmental: NA

3.4.2.3.5 Carcinogenesis: NA

3.4.2.3.6 Genetic and Related Cellular Effects Studies: NA

3.4.2.3.7 Other: Neurological, Pulmonary, Skin Sensitization, etc. Propane, used as an aerosol propellant with isobutane in deodorant and antiperspirant products (65–70% by weight), did not cause skin irritation in 125 volunteers who applied the aerosol products twice daily for 12 weeks (47).

3.5 Standards, Regulations, or Guidelines of Exposure

Propane is on the EPA TSCA Chemical Inventory and Test Submission Data Base (16). The immediately dangerous to life or health (IDLH) concentration established by NIOSH is 2,100 ppm, based on 10% of the lower explosion limit for safety considerations, even though the relevant toxicological data indicate that irreversible health effects or impairment of escape exist only at higher concentrations (36). The exposure limits for propane in the United States are listed in Table 49.2, and the international occupational limits are presented in Table 49.3.

Table 49.2. Occupational Exposure Limits for Propane in the United States[a]

Exposure Limits	OSHA PEL	NIOSH Exposure Limit	ACGIH TLV
Time-weighted average	1000 ppm (1800 mg/m^3)	1000 ppm (1800 mg/m^3)	2500 ppm (4508 mg/m^3)
Short-term exposure limit	—	—	—
Ceiling limit	—	—	—

[a]OSHA and ACGIH — 8-h TWA; NIOSH — 10-h TWA. From Ref. 19.

Table 49.3. Occupational Exposure Limits for Propane in Different Countries[a]

Country	Exposure Limit
Australia	Asphyxiant
Belgium	Asphyxiant
Denmark	TWA 1000 ppm (1800 mg/m^3)
Finland	TWA 800 ppm (1100 mg/m^3)
Germany	TWA 1000 ppm (1800 mg/m^3)
Hungary	Asphyxiant
The Netherlands	Asphyxiant
The Philippines	TWA 1000 ppm (1800 mg/m^3)
Switzerland	TWA 1000 ppm (1800 mg/m^3)
United Kingdom	Asphyxiant

[a]From Ref. 19.

4.0 *n*-Butane

4.0.1 CAS Number: [106-97-8]

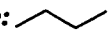
4.0.2 Synonyms: Diethyl, methylethyl methane; butane, methylethylmethane, butyl hydride, pyrofax

4.0.3 Trade Names: NA

4.0.4 Molecular Weight: 58.12

4.0.5 Molecular Formula: $CH_3(CH_2)_2CH_3$

4.0.6 Molecular Structure:



4.1 Chemical and Physical Properties

4.1.1 General

Butane, C_4H_{10}, is a flammable, colorless, and explosive gas, with specific gravity 0.6011. Butane occurs in natural gas and in the ambient urban air, in small concentrations. It has been detected in the exhaust of gasoline engines and in air above landfills and disposal sites (55, 56). Selected physical properties are listed in Table 49.1.

4.1.2 Odor and Warning Properties

Butane's odor can be detected between 2.9 and 14.6 mg/m^3 and in water at 6.2 ppm (21, 57).

ure, viscosity, surface
atic hydrocarbons are

exposures below the
m propane through the
en narcosis and lethal
plosive characteristics,
ffects may be accom-

pain, and occasionally
esthesia, and cardiac
e most common toxic
chemical pneumonitis
the oxygen in air is
ygen concentration is
is starved for oxygen.

with liquid aliphatic
n workers repeatedly
olvents and dissolve or
ing of the skin, that is,

the alveolar–capillary
e CNS depression, the
some alkanes have led
ne or *n*-hexane. Other
xylene, methyl ethyl
typewriter correction
nd exhaust emissions.
ng or memory impair-
and tachycardia (2–4).
corresponding parent
sic properties decrease
roperties increase with

natural gas; fire damp;

Table 49.1. Physicochemical Properties of Alkanes[a]

Compound	Molecular Formula	Molecular Weight	Boiling Point (°C)	Melting Point (°C)	Density (mg/cm^3) (at °C)	Refractive Index n_D	Solubility	Flash Point (°C)	Flammability limits (%)
Methane	CH_4	16.042	−161.5	−182.5	0.4228 (−162)	—	w 3, al 3, et 3, ac 2	−187.8 (open cup)	5.0–15.0
Ethane	C_2H_6	30.07	−88.63	−183.23	0.5446 (−89)	—	bz 4	−135	3.0–12.5
Propane	C_3H_8	44.09	−42.1	−187.7	0.493 (25)	—	w 3, al 3, et 4, ac 2	−104.0	2.1–9.5
Butane	C_4H_{10}	58.12	−0.5	−138.35	0.573 (25)	1.3326 (20)	w 3, al 4, et 4, ch 4	−60.0 (closed cup)	1.9–8.5
2-Methylpropane	C_4H_{10}	58.12	−11.7	−159.6	0.5510 (25)	1.3518 (−25)	w 2, al 3, et 3, ch 3	−82.8 (closed cup)	1.8–8.4
Pentane	C_5H_{12}	72.15	36.1	−129.8	0.6262 (20)	1.3575 (20)	w 2, al 5, et 5, ac 5	−49.0	1.4–8.0
2-Methylbutane	C_5H_{12}	72.15	27.8	−159.8	0.6201 (20)	1.3537 (20)	w 1, al 5, et 5	−51.0	1.4–7.6
2,2-Dimethylbutane	C_6H_{14}	86.177	49.7	−100	0.6444 (25)	1.3688 (20)	w 1, al 3, et 3, ac 4	−48.0	1.2–7.0
2,3-Dimethylbutane	C_6H_{14}	86.177	58	−128.5	0.6616 (20)	1.3750 (20)	w 1, al 3, et 3, ac 4	−29.0	1.2–7.0
2,2-Dimethylpropane	C_5H_{12}	72.15	9.5	−16.6	0.5258 (25)	1.3476 (6)	w 1, al 3, et 3, ct 3	−6.67	1.4–7.5
Hexane	C_6H_{14}	86.10	68.95	−95	0.6548 (25)	1.3749 (20)	w 1, al 4, et 3, ch 3	−22.0 (closed cup)	1.1–7.5
2-Methylpentane	C_6H_{14}	86.177	62	−154	0.650 (25)	1.3715 (20)	w 1, al 3, et 3, ac 5	−23.0	1.0–7.0
3-Methylpentane	C_6H_{14}	86.177	64	−118.0	0.6598 (25)	1.3765 (20)	w 1, al 3, et 5, ac 5	−6.0	1.2–7.0
Heptane	C_7H_{16}	100.20	98.4	−90.7	0.6837 (20)	1.3878 (20)	w 1, al 4, et 5, ac 5	−4.4 (closed cup)	1.05–6.7
2-Methylhexane	C_7H_{16}	100.20	90.0	−118.2	0.6787 (20)	1.3848 (20)	w 1, al 3, et 5, ac 5	−1.0	1.0–6.0
3-Methylhexane	C_7H_{16}	100.20	92.0	−119.0	0.6860 (20)	1.3887 (20)	w 1, al 3, et 5, ac 5	−4.0	—
Octane	C_8H_{18}	114.22	125.7	−56.8	0.6986 (25)	1.3974 (20)	w 1, al 3, et 3, ac 5	−13.0 (closed cup) 22 (open cup)	1.0–6.5

orl-man LDLo:4286 µg/kg/15H-I:CVS PGMJAO 60,155,84
orl-rat LD50:700 mg/kg ARZNAD 26,1849,76
ivn-rat LD50:18,800 µg/kg ARZNAD 26,1849,76
ivn-dog LD50:10 mg/kg ARZNAD 26,1849,76
SAFETY PROFILE: Poison by intravenous route. Moderately toxic by ingestion, subcutaneous, and intraperitoneal routes. Human systemic effects: paresthesia, wakefulness, hallucinations, distorted perceptions, pulse rate increase. Experimental reproductive effects. When heated to decomposition it emits toxic fumes of NO_x and HCl.

PMJ550 CAS: 57619-29-1 HR: 3
PRO-PAM
mf: $C_7H_{10}N_2O \cdot ClH$ mw: 174.65
SYNS: 1-METHYL-1,6-DIHYDROPICOLINALDEHYDE OXIME HYDROCHLORIDE □ N-METHYL-1,6-DIHYDROPYRIDINE-2-CARBALDOXIME HYDROCHLORIDE □ 1-METHYL-1,6-DIHYDRO-2-PYRIDINECARBOXYALDEHYDE OXIME HYDROCHLORIDE
TOXICITY DATA with REFERENCE:
ipr-mus LD50:173 mg/kg TXAPA9 47,305,79
ivn-mus LD50:168 mg/kg TXAPA9 47,305,79
ims-mus LD50:125 mg/kg TXAPA9 47,305,79
SAFETY PROFILE: Poison by intramuscular, intravenous, and intraperitoneal routes. When heated to decomposition it emits toxic fumes of NO_x and HCl.

PMJ750 CAS: 74-98-6 HR: 3
PROPANE
DOT: UN 1978
mf: C_3H_8 mw: 44.11
PROP: Colorless gas. Bp: −44.5°, flash p: −156°F, lel: 2.3%, uel: 9.5%, autoign temp: 842°F, d: 0.5852 @ −44.5°/4°, vap d: 1.56. Sol in water, alc, ether. IDLH 2100 ppm [10%LEL].
SYNS: DIMETHYLMETHANE □ PROPYL HYDRIDE
CONSENSUS REPORTS: Reported in EPA TSCA Inventory.
OSHA PEL: TWA 1000 ppm
DFG MAK: 1000 ppm (1800 mg/m³)
DOT CLASSIFICATION: 2.1; Label: Flammable Gas
SAFETY PROFILE: Central nervous system effects at high concentrations. An asphyxiant. Flammable gas. Highly dangerous fire hazard when exposed to heat or flame; can react vigorously with oxidizers. Explosive in the form of vapor when exposed to heat or flame. Explosive reaction with ClO_2. Violent exothermic reaction with barium peroxide + heat. To fight fire, stop flow of gas. When heated to decomposition it emits acrid smoke and irritating fumes.

PMK000 CAS: 542-78-9 HR: 2
PROPANEDIAL
mf: $C_3H_4O_2$ mw: 72.07
PROP: Hygroscopic needles. Mp: 72–74°.
SYNS: MALONALDEHYDE □ MALONDIALDEHYDE □ MALONIC ALDEHYDE □ MALONIC DIALDEHYDE □ MALONODIALDEHYDE □ MALONYLDIALDEHYDE □ NCI-C54842 □ 1,3-PROPANEDIAL □ 1,3-PROPANEDIALDEHYDE □ 1,3-PROPANEDIONE
TOXICITY DATA with REFERENCE:
mmo-sat 13,850 nmol/plate BTERDG 2,81,80
mmo-ese 2 mmol/L MUREAV 88,23,81
dnd-hmn:leu 1 mmol/L CLREAS 23(5),595A,75
mnt-rat:fbr 100 µmol/L MUREAV 101,237,82
skn-mus TDLo:7488 mg/kg/2Y-I:CAR AUODDK 55,3,80
skn-mus TD:30 g/kg/9W-I:CAR JNCIAM 53,1771,74
orl-rat LD50:632 mg/kg TXAPA9 7,826,65
orl-mus LD50:606 mg/kg AUODDK 55,3,80
CONSENSUS REPORTS: IARC Cancer Review: Group 3 IMEMDT 7,56,87; Animal Inadequate Evidence, IMEMDT 36,163,85. EPA Genetic Toxicology Program.
SAFETY PROFILE: Moderately toxic by ingestion. Questionable carcinogen with experimental carcinogenic data. Human mutation data reported. When heated to decomposition it emits acrid smoke and irritating fumes. See also ALDEHYDES.

PMK250 CAS: 78-90-0 HR: 3
1,2-PROPANEDIAMINE
DOT: UN 2258
mf: $C_3H_{10}N_2$ mw: 74.15
PROP: Flash p: 92°F (OC), d: 0.9, vap d: 2.6, bp: 118.9°.
SYNS: 1,2-DIAMINOPROPANE □ PROPYLENEDIAMINE □ PROPYLENE DIAMINE (DOT)
TOXICITY DATA with REFERENCE:
skn-rbt 10 mg/24H open AMIHBC 10,61,54
skn-rbt 435 mg open SEV UCDS** 3/12/69
eye-rbt 87 mg SEV UCDS** 3/12/69
orl-rat LD50:2230 mg/kg UCDS** 3/12/69
scu-rat LDLo:2250 mg/kg ZEPTAT 17,59,15
skn-rbt LD50:500 mg/kg AMIHBC 10,61,54
CONSENSUS REPORTS: Reported in EPA TSCA Inventory.
DOT CLASSIFICATION: 8; Label: Corrosive
SAFETY PROFILE: Moderately toxic by ingestion, skin contact, and subcutaneous routes. A corrosive irritant to eyes, skin, and mucous membranes. Dangerous fire hazard when exposed to heat, flames, oxidizers. To fight fire, use alcohol foam. When heated to decomposition it emits toxic fumes of NO_x. Used as an intermediate in production of petroleum and polymer additives, and surfactants. See also AMINES.

PMK500 CAS: 109-76-2 HR: 3
1,3-PROPANEDIAMINE
mf: $C_3H_{10}N_2$ mw: 74.15
PROP: Water-white liquid, amine odor. D: 0.8881 @ 20°/20°, fp: −12°, bp: 135–136°, flash p: 120°F (TOC). Completely sol in water, methanol, and ether.
SYNS: 1,3-DIAMINOPROPANE □ 1,3-PROPYLENEDIAMINE □ TRIMETHYLENEDIAMINE
TOXICITY DATA with REFERENCE:
skn-rbt 50 mg open SEV UCDS** 1/28/63
eye-rbt 1 mg SEV UCDS** 1/28/63
orl-rat LD50:350 mg/kg AIHAAP 23,95,62
skn-rbt LD50:200 mg/kg AIHAAP 23,95,62
CONSENSUS REPORTS: Reported in EPA TSCA Inventory.
SAFETY PROFILE: Poison by ingestion and skin contact. Experimental teratogenic effects. A severe skin

DFG, vol. 22 (2006)

資料P-13(DFG)

Propane

MAK value (1966)	**1000 ml/m³ (ppm) ≙ 1800 mg/m³**
Peak limitation (2002)	**Category II, excursion factor 2**
Absorption through the skin	–
Sensitization	–
Carcinogenicity	–
Prenatal toxicity (1994)	**see Section IIc of the *List of MAK and BAT Values***
Germ cell mutagenicity	–
BAT value	–
Synonyms	dimethyl methane *n*-propane
Chemical name	*n*-Propane
CAS number	74-98-6
Structural formula	C_3H_8, $CH_3\ CH_2\ CH_3$
Molecular weight	44.10
Melting point	187 C (BUA 1994)
Boiling point at 1013 hPa	42 C (ECB 2000)
Vapour pressure at 20 C	8340 hPa (BUA 1994)
log P_{ow}*	2.36 (BUA 1994)
1 ml/m³ (ppm) ≙ 1.83 mg/m³	**1 mg/m³ ≙ 0.55 ml/m³ (ppm)**

The MAK value for propane was established in 1966 in analogy to the TLV value at the time. This documentation is based on reviews of the toxicological data for propane (ACGIH 2001, BUA 1994, ECB 2000).

* *n*-octanol/water distribution coefficient

The MAK-Collection Part I: MAK Value Documentations, Vol. 22. DFG, Deutsche Forschungsgemeinschaft

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1 Toxic Effects and Mode of Action

Propane can be absorbed via inhalation. Dermal penetration is minimal.

In animal experiments propane was found to be slightly acutely toxic. Exposure to high concentrations of propane caused central nervous depression or even narcosis and increased sensitivity of the heart muscle to adrenaline.

Propane is not irritating in the eye or on the skin. Liquefied propane can cause "chemical freezing".

The available studies have not shown propane to be mutagenic.

There are no data available for the mechanism of action of propane.

2 Toxicokinetics and Metabolism

In mice, propane was metabolised to isopropanol and acetone following pulmonary absorption. After inhalation of 50000 ml/m^3 propane during one hour, the two metabolites were detected in the blood, liver, kidneys and brain. When incubated *in vitro* with mouse liver microsomes, propane was metabolised to isopropanol and further oxidised to acetone (BUA 1994).

3 Effects in Humans

There are no data available for the allergenic effects of propane in humans, or its genotoxicity, reproductive toxicity and carcinogenicity.

3.1 Single exposures

Two accidents with direct skin contact have been reported with propane. Erythema, oedema and deep necroses occurred as a result of frostbite (James and Moss 1989).

3.2 Repeated exposures

In a double-blind study 1 or 2 volunteers were exposed to a mixture of isobutane/propane with a propane concentration of 77, 102 or 107 ppm (141, 187 or 196 mg/m^3) for 1 to 2 hours or 4 volunteers were exposed to a mixture with a propane concentration of 100,

962 or 1030 ppm (183, 1760 or 1885 mg/m³) for eight hours during two days. No clinical symptoms associated with the exposure could be detected, nor were effects in the electrocardiogram (ECG), effects in the electroencephalogram or pulmonary dysfunctions observed. All haematological parameters examined were within the normal range (Stewart *et al.* 1977).

22 workers from a liquid gas filling station (propane and butane), who were exposed to a maximum of 0.8 volume parts gas (8000 ml/m³) (measurements carried out on two occasions), reported symptoms such as dry throat, dry cough, severe agitation and sometimes dizziness. One worker complained of precordialgia, tachycardia, eructation and stomach pains. Medical examination revealed breathing difficulties, shortness of breath and tachycardia in some workers, at times coupled with irregular heartbeat (arrhythmia) and pains in the epigastric angle. ECG examination of the workers revealed tachycardia and arrhythmia (BUA 1994).

One case history concerns the driver of a propane gas transporter who was diagnosed as having a primary hepatic lymphoma. However, this could not be unequivocally attributed to propane gas (BUA 1994).

3.3 Local effects on skin and mucous membranes

Gaseous propane does not have irritative effects on the skin or eyes. Direct contact with liquefied propane can cause corrosive lesions und "chemical freezing" (James and Moss 1989, Sandmeyer 1981).

4 Animal Experiments and *in vitro* Studies

There are no data available for local effects of propane on skin and mucous membranes of animals. Nor is there information on allergenic effects, reproductive toxicity or carcinogenicity.

4.1 Acute toxicity

Inhalation

According to studies with single exposures, the acute toxicity of propane is very weak. The LC_{50} of propane for rats after exposure for 15 minutes was found to be > 800000 ml/m³ (80%; 1464000 mg/m³); the EC_{50} (CNS) after 10-minute exposure was 280000 ml/m³ (28%; 512400 mg/m³). Acute inhalation exposure to propane led to central nervous symptoms such as limb tremor, ataxia, loss of righting reflex, narcosis,

convulsions and death due to respiratory depression (BUA 1994). The exposure of dogs to propane concentrations of 100000 ml/m³ (10%) for 5 minutes caused sensitization of the heart muscle to adrenaline. The EC_{50} for heart muscle sensitization caused by exposure for 5 minutes was found to be 180000 ml/m³ (18%; 329400 mg/m³) (Clark and Tinson 1982).

The exposure of rhesus monkeys to 100000 ml/m³ propane caused a suppressed breathing rate. No other symptoms were seen. Information about the duration of exposure was not provided (Aviado 1975).

4.2 Subacute, subchronic and chronic toxicity

Inhalation

Inhalation exposure of 21 cynomolgus monkey to 750 ml/m³ of a deodorant (> 50 % propane) for 90 days resulted in no symptoms related to the exposure (Anonymous 1982).

4.3 Genotoxicity

Propane (5, 10, 20, 30 40 and 50 % (v/v) in air) was non-mutagenic, both with and without metabolic activation, in a *Salmonella* mutagenicity test that had been modified for the investigation of gases and performed with the strains TA98, TA100, TA1535, TA1537 and TA1538 (Kirwin and Thomas 1980).

A mixture of about 25% each of propane and isobutane was tested with yeast (0.005, 0.01, 0.05, 0.1, 0.25, 0.5 and 1 % corresponding to 0.229 to 45.75 mg/m³). The mixture was found to be non-mutagenic; concentrations of 0.5 % and 1 % were cytotoxic (ECB 2000).

5 Manifesto (MAK value/classification)

Propane causes depression of the central nervous system after inhalation in high concentrations. There are no data available for the effect threshold in humans and useful studies with experimental animals are lacking.

Exposure of volunteers to a propane concentration of 1000 ml/m³, the present MAK value, on two consecutive days revealed no effects. The studies are of limited significance due to the small number of persons. In 1999 a MAK value of 1000 ml/m³ was established for *n*-butane (see documentation in Volume 20 of present series). Therefore, the present MAK value for propane of 1000 ml/m³ (1800 mg/m³) can be

retained. The category II for the limitation of exposure peaks with an excursion factor of 2 can also be retained.

Due to lack of data for toxic effects of propane on reproduction, the substance is listed in Section IIc of the *List of MAK and BAT Values.* Because data are inadequate, propane is not designated with "H" (for substances for which there is danger from cutaneous absorption) or "Sa" or "Sh" (for substances which cause sensitization).

The germ cell mutagenic potential of propane has to date not been investigated and cannot, therefore, be evaluated.

7 References

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Sandmeyer EE (1981) Aliphatic hydrocarbons. in: Clayton GD, Clayton FE (Eds) *Patty's Industrial Hygiene and Toxicology*, Vol 2B, John Wiley & Sons, New York, 3175–3220

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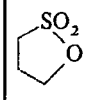
completed 26.06.2003

Substance [CAS number]	Formula	MAK ml/m³ (ppm)	MAK mg/m³	Peak limitation	H;S	Carcinogen category	Pregnancy risk group	Germ cell mutagen categ.	Vapour pressure in hPa at 20°C
Propane [74-98-6]	$H_3C-CH_2-CH_3$	1000	1800	II(4)			D		
1,2-Propanediol	see Propylene glycol								
1,3-Propane sultone [1120-71-4]		–	–	–	H	2	–		
1,2,3-Propanetriol	see Glycerin								
2-Propanol	see Isopropyl alcohol								
Propargyl alcohol [107-19-7]	$HC\equiv C-CH_2OH$	2	4.7	I(2)	H		D		11.6
2-Propenal	see Acrolein								
2-Propenoic acid 1,4-butanediyl ester	see 1,4-Butanediol diacrylate								
2-Propenoic acid 1,2-ethanediylbis(oxy-2,1-ethanediyl)ester	see Triethylene glycol diacrylate								
2-Propenoic acid homopolymer	see Acrylic acid polymer								
2-Propenoic acid 2-hydroxyethyl ester	see Acrylic acid 2-hydroxyethyl ester								
2-Propenoic acid 2-(hydroxymethyl)-2-(((1-oxo-2-propenyl)oxy)-methyl)-1,3-propanediyl ester	see Pentaerythritol triacrylate								
2-Propenoic acid hydroxypropyl ester	see Acrylic acid hydroxypropyl ester								
2-Propenoic acid oxydi-2,1-ethanediyl ester	see Diethylene glycol diacrylate								
2-Propen-1-ol	see Allyl alcohol								
4-Propenyl-2-methoxyphenol	see Isoeugenol								
β-Propiolactone [57-57-8]		–	–	–	H	2	–		

Chemical Name Formula (Synonym) CAS No.	NFPA 30/ OSHA Class	Flash Point °F(°C)	Ignition Temp. °F(°C)	Flammable Limits Percent by Vol. Lower	Upper	Sp.Gr. (Water =1)	Vapor Density (Air =1)	Boiling Point °F(°C)	Water Soluble	Extinguishing Methods	Hazard Identification Health	Flammability	Instability
Polyamyl Naphthalene		380 (182) (oc)				0.9		667–747 (353–397)	No	2	0	1	0
Polyethylene Glycols $OH(C_2H_4O)_nC_2H_4OH$ 25322-68-3		350–550 (162–287) (oc)							Yes	5 2	1	1	0
Polyoxyethylene Lauryl Ether $C_{12}H_{25}O(OCH_2CH_2)_nOH$ 9002-92-0	IIIB	>200 (>93)				0.95					0	1	0
Polypropylene Glycols $OH(C_3H_6O)_nC_3H_6OH$ 25322-69-4		385 (185) (oc)				1.0+		Decomposes		5 2	0	1	0
Polyvinyl Alcohol 9002-89-5		175 (70) (oc)							Yes	5	0	2	0
Poppy Seed Oil	IIIB	491 (255)				0.9			No	2	0	1	0
Potassium Xanthate $KS_2C\text{-}OC_2H_5$ 140-89-6	IIIB	205 (96)			9.6	1.56	5.53	392 (200) Decomposes	Yes		1	1	0
Propanal	See Propionaldehyde.												
Propane $CH_3CH_2CH_3$ 74-98-6		Gas	842 (450)	2.1	9.5		1.6	−44 (−42)	No	6	2	4	0
1,3-Propanediamine $NH_2CH_2CH_2CH_2NH_2$ (1,3-Diaminopropane) (Trimethylenediamine) 109-76-2		75 (24) (oc)				0.9	2.6	275 (136)	Yes	1 5	3	3	0
1,2-Propanediol	See Propylene Glycol.												
1,3-Propanediol	See Trimethylene Glycol.												
1-Propanol	See Propyl Alcohol.												
2-Propanol	See Isopropyl Alcohol.												
2-Propanone	See Acetone.												
Propanoyl Chloride	See Propionyl Chloride.												
Propargyl Alcohol $HC{\equiv}CCH_2OH$ (2-Propyn-1-ol) 107-19-7	Note: May polymerize explosively. See NFPA 49 contained in this guide.	97 (36) (oc)				0.97	1.93	239 (115)	Yes	1	4	3	3
Propene	See Propylene.												
2-Propenylamine	See Allylamine.												
Propenyl Ethyl Ether $CH_3CH{:}CHOCH_2CH_3$ 926-65-2		<20 (<−7) (oc)				0.8	1.3	158 (70)		1	2	3	0
β-Propiolactone $C_3H_4O_2$ 57-57-8	IIIA	165 (74)		2.9		1.1	2.5	311 (155)	Yes	5	0	2	0
Propionaldehyde CH_3CH_2CHO (Propanal) 123-38-6	IB	−22 (−30)	405 (207)	2.6	17	0.8	2.0	120 (49)	Slight	1 5	2	3	2
	See NFPA 49 contained in this guide.												
Propionic Acid CH_3CH_2COOH 79-09-4	II	126 (52)	870 (465)	2.9	12.1	1.0−	2.5	297 (147)	Yes	5	3	2	0
	See NFPA 49 contained in this guide.												

NFPA, 2002

CRC, 2004

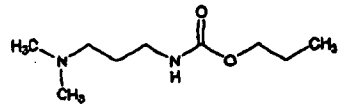
PHYSICAL CONSTANTS OF ORGANIC COMPOUNDS (continued)

No.	Name	Synonym	Mol. Form.	CAS RN	Mol. Wt.	Physical Form	mp/°C	bp/°C	den/g cm⁻³	n_D	Solubility
9119	Prodiamine		$C_{13}H_{17}F_3N_4O_4$	29091-21-2	350.294		124		1.47^{25}		
9120	Profenofos		$C_{11}H_{15}BrClO_3PS$	41198-08-7	373.631			$110^{0.001}$	1.455^{20}		
9121	Profluralin		$C_{14}H_{16}F_3N_3O_4$	26399-36-0	347.290		34				
9122	Progesterone	Pregn-4-ene-3,20-dione	$C_{21}H_{30}O_2$	57-83-0	314.462	pr	129		1.166^{23}		i H_2O; s EtOH, diox, ace
9123	*DL*-Proline		$C_5H_9NO_2$	609-36-9	115.131	hyg nd (al-eth) cry (+w)	205 dec				vs H_2O, EtOH
9124	*L*-Proline	2-Pyrrolidinecarboxylic acid	$C_5H_9NO_2$	147-85-3	115.131	nd (al-eth) pr (w)	221 dec				vs H_2O; sl EtOH, ace, bz; i eth, PrOH
9125	Promazine		$C_{17}H_{20}N_2S$	58-40-2	284.419			$206^{0.3}$			
9126	Promecarb	Phenol, 3-methyl-5-(1-methylethyl)-, methylcarbamate	$C_{12}H_{17}NO_2$	2631-37-0	207.269		87	$117^{0.01}$			
9127	Promethazine	*N,N*,α-Trimethyl-10*H*-phenothiazine-10-ethanamine	$C_{17}H_{20}N_2S$	60-87-7	284.419		60	$191^{0.5}$			i H_2O; vs dil HCl
9128	Promethazine hydrochloride	Diprazin	$C_{17}H_{21}ClN_2S$	58-33-3	320.880		231				vs H_2O, EtOH, chl
9129	Prometone		$C_{10}H_{19}N_5O$	1610-18-0	225.291	solid	91.5				
9130	Prometryn	*N,N'*-Diisopropyl-6-(methylthio)-1,3,5-triazine-2,4-diamine	$C_{10}H_{19}N_5S$	7287-19-6	241.357		119		1.157^{20}		
9131	Propachlor	Acetamide, 2-chloro-*N*-(1-methylethyl)-*N*-phenyl-	$C_{11}H_{14}ClNO$	1918-16-7	211.688		77	$110^{0.03}$	1.242^{25}		
9132	Propanal	Propionaldehyde	C_3H_6O	123-38-6	58.079	liq	-80	48	0.8657^{25}	1.3636^{20}	s H_2O; msc EtOH, eth
9133	Propanal oxime		C_3H_7NO	627-39-4	73.094		40	131.5	0.9256^{20}	1.4287^{20}	
9134	Propanamide	Propionamide	C_3H_7NO	79-05-0	73.094	rhom, pl (bz)	81.3	213	0.9262^{110}	1.4180^{110}	vs H_2O, EtOH, eth, chl
✓9135	Propane		C_3H_8	74-98-6	44.096	col gas	-187.63	-42.1	0.493^{25} (p>1 atm)		s H_2O, EtOH; vs eth, bz; sl ace
9136	Propanediamide		$C_3H_6N_2O_2$	108-13-4	102.092	mcl pr(w)	170.8				s H_2O; i EtOH, eth, bz; sl DMSO
9137	1,2-Propanediamine, (±)	Propylenediamine	$C_3H_{10}N_2$	10424-38-1	74.124	hyg		119.5	0.878^{15}	1.4460^{20}	vs H_2O; i eth; vs chl
9138	1,3-Propanediamine	1,3-Diaminopropane	$C_3H_{10}N_2$	109-76-2	74.124	liq	-10.8	139.8	0.884^{25}	1.4600^{20}	s H_2O; msc EtOH, eth
9139	1,2-Propanediol diacetate		$C_7H_{12}O_4$	623-84-7	160.168			190.5	1.059^{20}	1.4173^{20}	vs H_2O; s EtOH, eth
9140	1,3-Propanediol diacetate		$C_7H_{12}O_4$	628-66-0	160.168			209.5	1.070^{14}	1.4192	vs H_2O; s EtOH
9141	1,2-Propanediol 1-methacrylate	2-Hydroxypropyl methacrylate	$C_7H_{12}O_3$	923-26-2	144.168			90^9, $57^{0.5}$	1.066^{25}	1.4458^{20}	
9142	1,2-Propanedione	Pyruvaldehyde	$C_3H_4O_2$	78-98-8	72.063	ye hyg liq		72	1.0455^{20}	1.4002^{18}	s EtOH, eth, bz
9143	Propanedioyl dichloride		$C_3H_2Cl_2O_2$	1663-67-8	140.953			57^{28}	1.4509^{20}	1.4639^{20}	s eth, AcOEt
9144	1,2-Propanedithiol		$C_3H_8S_2$	814-67-5	108.226			152	1.08^{20}	1.532^{20}	s chl
9145	1,3-Propanedithiol	Trimethylene dimercaptan	$C_3H_8S_2$	109-80-8	108.226	liq	-79	172.9	1.0772^{20}	1.5392^{20}	sl H_2O, ctc; msc EtOH, eth, bz
9146	2,2'-[1,3-Propanediylbis(nitrilomethylidyne)]bisphenol	Disalicylidene-1,3-propanediamine	$C_{17}H_{18}N_2O_2$	120-70-7	282.337		54.3				
9147	Propanenitrile	Ethyl cyanide	C_3H_5N	107-12-0	55.079	liq	-92.78	97.14	0.7818^{20}	1.3655^{20}	vs H_2O; s EtOH, eth, ace, bz, ctc
9148	1-Propanesulfonic acid		$C_3H_8O_3S$	5284-66-2	124.159		8	136^1	1.2518^{25}		
9149	1-Propanesulfonyl chloride		$C_3H_7ClO_2S$	10147-36-1	142.605			dec 180; 77^{12}	1.267^{20}	1.452^{20}	
9150	1,3-Propane sultone	1,2-Oxathiolane, 2,2-dioxide	$C_3H_6O_3S$	1120-71-4	122.143						s chl
9151	1-Propanethiol	Propyl mercaptan	C_3H_8S	107-03-9	76.161	liq	-113.13	67.8	0.8411^{20}	1.4380^{20}	sl H_2O; s EtOH, eth, ace, bz
9152	2-Propanethiol	Isopropyl mercaptan	C_3H_8S	75-33-2	76.161	liq	-130.5	52.6	0.8143^{20}	1.4255^{20}	sl H_2O; msc EtOH, eth; vs ace; s chl
9153	1,2,3-Propanetriamine	1,2,3-Triaminopropane	$C_3H_{11}N_3$	21291-99-6	89.139	visc oil		190; 92^9			s H_2O
9154	1,2,3-Propanetricarboxylic acid	Tricarballylic acid	[illegible]	99-14-9	176.124	orth (eth)	166				vs H_2O, EtOH; sl eth

THERAP CAT: Antiprotozoal (Trypanosoma); antiamebic.

THERAP CAT (VET): Anti-infective (topical). Formerly used as antiprotozoal (Trypanosoma, Babesia).

7798. Propamocarb. [24579-73-5] [3-(Dimethylamino)-propyl]carbamic acid propyl ester; propyl-(3-dimethylaminopropyl) carbamate. $C_9H_{20}N_2O_2$; mol wt 188.27. C 57.42%, H 10.71%, N 14.88%, O 17.00%. Systemic carbamate fungicide. Prepn: BE 708057 (1968 to Schering AG). Prepn of salts: G.-A. Hoyer, E. A. Pieroh, US 3649674 (1972 to Schering AG). Properties and activity: E. A. Pieroh *et al., Meded. Fac. Landbouwwet. Rijksuniv. Gent* 43, 933 (1978). Metabolic fate in bluegills and catfish: C. Gray, C. O. Knowles, *Chemosphere* 10, 469 (1981). Efficacy vs late blight fungus on potato: Y. Samoucha, Y. Cohen, *Phytoparasitica* 18, 27 (1990). GC determn in food products: T. Nagayama *et al., J. AOAC Int.* 79, 769 (1996). Uptake and redistribution in potato and grapevine: R. L. Harris, *Brighton Crop Prot. Conf. - Pests Dis.* 1996, 281.



bp_{18mm} 139-141°. n_D^{20} 1.4490.

Hydrochloride. [25606-41-1] SN-66752; AE-B066752; HOE-102791; Banol; Previcur; Proplant. $C_9H_{20}N_2O_2.HCl$; mol wt 224.73. Colorless, odorless crystals, mp 45-55°. Soly at 25° (g/100ml): water >70; dichloromethane >43; methanol >50. Vapor pressure at 25°: 6×10^{-6} torr. LD_{50} orally in rats: 8600 mg/kg. LC_{50} (96 hr) in rainbow trout, sunfish, carp (ppm): 616, 415, 234 (Pieroh).

USE: Agricultural fungicide.

7799. Propane. [74-98-6] Dimethylmethane; propyl hydride. C_3H_8; mol wt 44.10. C 81.71%, H 18.28%. $CH_3CH_2CH_3$. Constituent of natural gas and of crude petroleum. Obtained by the so-called "stabilization process" using fractional distillation under pressure: Francis, Robbins, *J. Am. Chem. Soc.* 55, 4339 (1933). Many syntheses, e.g., by using butyronitrile and sodium: Timmermans, *J. Chim. Phys.* 18, 133 (1920).

Gas. Odorless when pure. Burns with a luminous, smoky flame. Explosive limits, % by vol in air: 2.37-9.5. Heavier than air. One liter weighs 2.0200 g at 0° and 760 mm; 1.8324 g at 25° and 760 mm. Liquefies at -42°; solid at -187.7°. bp (1 atm) -42.1°; bp (2 atm) -25.6°; bp (5 atm) 1.4°; bp (10 atm) 26.9°; bp (20 atm) 58.1°; bp (30 atm) 78.7°; bp (40 atm) 94.8°. Crit temp 96.81°; crit press. 42.01 atm. Heat of combustion (const vol) 528.4 cal, (const pressure) 553.5 cal. 100 vols water dissolve 6.5 vols at 17.8° and 753 mm pressure; 100 vols abs alc dissolve 790 vols at 16.6° and 754 mm pressure; 100 vols ether dissolve 926 vols at 16.6° and 757 mm pressure; 100 vols chloroform dissolve 1299 vols at 21.6° and 757 mm pressure; 100 vols benzene dissolve 1452 vols at 21.5° and 757 mm pressure; 100 vols turpentine dissolve 1587 vols at 17.7° and 757 mm pressure.

Caution: Potential symptoms of overexposure are dizziness, confusion, excitation, asphyxia; direct contact with liquid may cause frostbite. *See NIOSH Pocket Guide to Chemical Hazards* (DHHS/-NIOSH 97-140, 1997) p 262.

USE: As fuel gas, sometimes mixed with butane. In organic syntheses. As refrigerant.

7800. 1-Propanearsonic Acid. [107-34-6] *n*-Propylarsonic acid. $C_3H_9AsO_3$; mol wt 168.02. C 21.45%, H 5.40%, As 44.59%, O 28.57%. $C_3H_7AsO(OH)_2$.

White needles, mp 125°. Freely sol in water; sol in alcohol. Insol in ether.

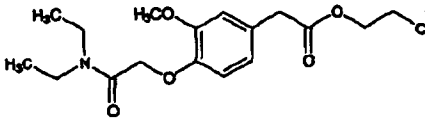
USE: For the determination of zirconium.

7801. 1,3-Propanedithiol. [109-80-8] 1,3-Dimercaptopropane; trimethylenedithioglycol; dithiotrimethyleneglycol; trimethylenedimercaptan. $C_3H_8S_2$; mol wt 108.23. C 33.29%, H 7.45%, S 59.25%. $HSCH_2CH_2CH_2SH$. Prepd by alkaline hydrolysis of propylene-1,3-diisothiuronium dihydrochloride: Grogan *et al., J. Org. Chem.* 20, 50 (1955).

Oil. Disagreeable odor. d_4^{20} 1.0772. bp_{760} 169-170°; bp_{759} 170-171°; bp_{56} 92-98°. n_D^{20} 1.5392. Volatile with steam. Slightly sol in water. Miscible with alcohol, ether, chloroform and benzene.

7802. Propanethial *S*-Oxide. [32157-29-2] Thiopropionaldehyde *S*-oxide; thiopropanal *S*-oxide. C_3H_6OS; mol wt 90.14, C 39.97%, H 6.71%, O 17.75%, S 35.57%. $CH_3CH_2CH{=}$ Lachrymatory factor of the onion, *Allium cepa L.*, found as a *cis*- and 5% *trans*- mixture. Early structure studies: W. D. Virtanen, *Acta Chem. Scand.* 17, 641 (1963). Structure: Brodnitz, J. V. Pascale, *J. Agric. Food Chem.* 19, 269 (1971). Stereochemistry: E. Block *et al., J. Am. Chem. Soc.* 101, (1979); *eidem, Tetrahedron Lett.* 21, 1277 (1980). Chemistry: *eidem, J. Am. Chem. Soc.* 102, 2490 (1980).

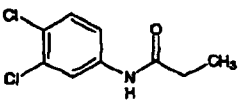
7803. Propanidid. [1421-14-3] 4-[2-(Diethylamino)-2-oxoethoxy]-3-methoxybenzeneacetic acid propyl ester; [4-[(diethylcarbamoyl)methoxy]-3-methoxyphenyl]acetic acid propyl ester; methoxy-4-[(*N*,*N*-diethylcarbamido)methoxy]phenyl]acetic acid propyl ester; propyl [4-[(diethylcarbamoyl)methoxy]-3-methoxyphenyl]acetate; Bayer 1420; FBA-1420; Epontol; Sombrevin. $C_{17}H_{27}NO_5$; mol wt 337.41. C 64.07%, H 8.07%, N 4.15%, O 23.[illegible]. Prepn: R. Hiltmann *et al.*, DE 1134981; US 3086978 (1962, both to Bayer). Toxicity study: E. I. Goldenthal, *Toxicol. Pharmacol.* 18, 185 (1971).



Pale yellow oil, $bp_{0.7}$ 210-212°. Practically insol in water; [illegible] alcohol, chloroform. LD_{50} orally in rats: >10,000 mg/kg (Goldenthal).

THERAP CAT: Anesthetic (intravenous).

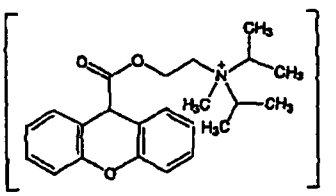
7804. Propanil. [709-98-8] *N*-(3,4-Dichlorophenyl)propanamide; 3',4'-dichloropropionanilide; *N*-(3,4-dichlorophenyl)propionamide; DPA; FW-734; Stam; Stampede. $C_9H_9Cl_2NO$; mol wt 218.08. C 49.57%, H 4.16%, Cl 32.51%, N 6.42%, O 7.[illegible]. Selective contact herbicide. Prepn: W. Schäfer *et al.*, DE 10[illegible] (1958 to Bayer), *C.A.* 54, 20060l (1960); Huffman, Allen, *J. Agric. Food Chem.* 8, 298 (1960). Use in nematocide formulation: Fielding, Stoddard, US 3108038 (1963 to du Pont). Toxicity: G. W. Bailey, J. L. White, *Residue Rev.* 10, 97 (1965).



White crystalline solid, mp 91-93°. Soly in water at room [illegible] 225 ppm. LD_{50} orally in rats: 1384 mg/kg (Bailey, White).

USE: Herbicide.

7805. Propantheline Bromide. [50-34-0] *N*-Methyl-*N*-methylethyl-*N*-[2-[(9*H*-xanthen-9-ylcarbonyl)oxy]ethyl]-2-propanaminium bromide; (2-hydroxyethyl)diisopropylmethylammonium bromide xanthene-9-carboxylate; β-diisopropylaminoethyl 9-thenecarboxylate methobromide; Corrigast; Ercotina; Pro-Banthine; Neo-Metantyl; Pantheline. $C_{23}H_{30}BrNO_3$; mol wt 448.[illegible] 61.61%, H 6.74%, Br 17.82%, N 3.12%, O 10.70%. Synthetic quaternary ammonium anticholinergic. Prepn: Cusic, Robinson, *J. Org. Chem.* 16, 1921 (1951); US 2659732 (1953 to Searle). Metabolic studies: Beermann *et al., Clin. Pharmacol. Ther.* 212 (1972).



Crystals from isopropanol + ether, mp 159-161°. Very soluble in water, alcohol, chloroform. Practically insol in ether, benzene.

Merck, 2006

資料P-18(NIOSH PG)

Propane

NIOSH Pocket Guide

1.0 CHEMICAL NAME, STRUCTURE/FORMULA, CAS AND RTECS NOS., AND DOT ID AND GUIDE NOS.▲

Chemical Name: Propane

Formula: $CH_3CH_2CH_3$

Structure/Formula: $CH_3CH_2CH_3$

CAS Number: 74-98-6

RTECS Number: TX2275000

DOT ID and NAERG Guide Numbers: 1075 115
1978 115

2.0 SYNONYMS, TRADENAMES AND CONVERSION FACTORS▲

Synonyms/Tradenames: Bottled gas; Dimethyl methane; n-Propane; Propyl hydride

Conversion Factor at 68° F and 760 mmHg: 1 ppm = 1.80 mg/m^3

3.0 EXPOSURE LIMITS (TWA UNLESS NOTED OTHERWISE)▲

NIOSH Recommended Exposure Limits (RELs): Time-weighted average (TWA) 1000 ppm (1800 mg/m^3)

OSHA Permissible Exposure Limits (PELs): Time-weighted average (TWA) 1000 ppm (1800 mg/m^3)

4.0 IDLH▲

2100 ppm [The IDLH was based on 10% of the lower explosive limit for safety considerations even though the revelant toxicological data indicated that irreversible health effect or impairment of escape existed only at higher concentrations.]

5.0 PHYSICAL DESCRIPTION▲

Colorless, odorless gas.

Notes: [A foul-smelling odorant is often added when used for fuel purposes. Shipped as a liquefied compressed gas.]