converted to sinus tachycardia. He had generalised tonic clonic seizures, treated with diazepam, phenytoin and phenobarbitone. It was determined by ECG that he had suffered an anterolateral MI and was treated with dobutamine and captopril. CT scan showed bilateral hemispheric infarcts. He was ventilated for 13 days. During his hospital admission his cardiac status improved but he suffered memory and personality problems at the time of discharge (Bauman et al., 1991)).

Hemiparesis

A 15 year old boy inhaled half a can of butane then fell to the ground with his right leg 'dead'. On examination he was alert and orientated with a marked right sided hemiparesis, power was reduced to grade 1/5 in both arm and leg. Within 24 hours the power in the right hand and forearm was grade 3/5 and he was able to stand with assistance. On discharge 5 days later he had pronounced upper limb proximal muscle weakness and hemiplegic gait. CT scan was normal (Gray and Lazarus, 1993).

12. Additional information

12.1 Specific preventive measures

12.2 Other

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14. AUTHOR(S), REVIEWER(S), DATE(S) (INCLUDING UPDATES), COMPLETE ADDRESS(ES)

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Editor: Dr M.Ruse (September, 1998)

See Also:
Toxicological Abbreviations
BUTANE (JECFA Evaluation)

資料B-11(CHRIS)

BUTANE

CHRIS – Chemical Hazard Response Information System

0. OVERVIEW

Material name

BUTANE
CHRIS Code BUT

Common synonyms

n-Butane

Characteristics

Liquefied compressed gas Colorless Gasoline-like odor
Floats and boils on water. Flammable, visible vapor cloud is formed.

Emergency Actions

Restrict access.
Evacuate.
Shut off ignition sources and call fire department.
Stay upwind and use water spray to ``knock down'' vapor.
Avoid contact with liquid and vapor.
Notify local health and pollution control agencies.
Protect water intakes.

Fire

FLAMMABLE.
Flashback along vapor trail may occur.
Vapor may explode if ignited in an enclosed area.
Stop flow of gas if possible.
Cool exposed containers and protect men effecting shut-off with water.
Let fire burn.

Exposure

CALL FOR MEDICAL AID.
VAPOR
If inhaled, will cause dizziness or difficult breathing.
Not irritating to eyes, nose or throat.
Move to fresh air.
If breathing has stopped, give artificial respiration.
If breathing is difficult, give oxygen.
LIQUID
Will cause frostbite.
Flush affected areas with plenty of water.
DO NOT RUB AFFECTED AREAS.

Water Pollution - General

Not harmful to aquatic life.
May be dangerous if it enters water intakes.
Notify operators of nearby water intakes.

1. CORRECTIVE RESPONSE ACTIONS

Stop discharge
Chemical and Physical Treatment: Burn

2. CHEMICAL DESIGNATIONS

CG Compatibility Group: 31; Paraffin
Formula: $n-C^4H^{10}$
IMO/UN Designation: 2.0/1011
DOT ID Number: 1011
CAS Registry Number: 106-97-8
NAERG Guide Number: 115
Standard Industrial Trade Classification: 51114

3. HEALTH HAZARDS

Personal Protective Equipment: Self-contained breathing apparatus and safety goggles.
Symptoms Following Exposure: High exposure produces drowsiness but no other evidence of systemic effect.
Treatment of Exposure: ORAL AND ASPIRATION: No treatment required. INHALATION: Guard against self-injury if stuporous, confused, or anesthetized. Apply artificial respiration if not breathing. Avoid administration of epinephrine or other sympathomimetic amines. Prevent aspirations of vomitus by proper positioning of the head. Give symptomatic and supportive treatment.
TLV-TWA: 800 ppm
TLV-STEL: Not listed.
TLV-Ceiling: Not listed.
Toxicity by Ingestion: Not pertinent
Toxicity by Inhalation: Currently not available.
Chronic Toxicity: None
Vapor (Gas) Irritant Characteristics: None
Liquid or Solid Irritant Characteristics: No appreciable hazard. Practically harmless to the skin because it is very volatile and evaporates quickly from the skin. Some frostbite possible.
Odor Threshold: 6.16 ppm
IDLH Value: Not listed.
OSHA PEL-TWA: Not listed.
OSHA PEL-STEL: Not listed.
OSHA PEL Ceiling: Not listed.
EPA AEGL: Not listed.

4. FIRE HAZARDS

Flash Point: −76° F C.C.
Flammable Limits in Air: 1.8%-8.4%
Fire Extinguishing Agents: Stop flow of gas

Fire Extinguishing Agents NOT to Be Used: Not pertinent
Special Hazards of Combustion Products: Not pertinent
Behavior in Fire: Not pertinent
Ignition Temperature: 550° F
Electrical Hazard: Class 1, Group D
Burning Rate: 7.9 mm/min.
Adiabatic Flame Temperature: 2435. (Est.)
Stoichiometric Air to Fuel Ratio: 30.9 (calc.)
Flame Temperature: Currently not available
Combustion Molar Ratio (Reactant to Product): 9.0 (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: 99.95%; Pure: 99.4%; Technical: 97.6%
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: 58.12

Boiling Point at 1 ATM: 31.1° F = −0.48° C = 272.72° K

Freezing Point: −216° F = −138° C = 135° K

Critical Temperature: 306° F = 152° C = 425° K

Critical Pressure: 550.8 psia = 37.47 atm = 3.796 MN/m^2

Specific Gravity: 0.60 at 0° C (liquid)

Liquid Surface Tension (Est.): 14.7 dynes/cm = .0147 N/m at 0° C

Liquid Water Interfacial Tension: (est.) 65 dynes/cm = 0.065 N/m at 22° C

Vapor (Gas) Specific Gravity: 2 at 20° C

Ratio of Specific Heats of Vapor (Gas): 1.092

Latent Heat of Vaporization: 170 Btu/lb = 92 cal/g = 3.9 X 10^5 J/kg

Heat of Combustion: −19,512 Btu/lb = −10,840 cal/g = −453.85 X 10^5 J/kg

Heat of Decomposition: Not pertinent

Heat of Solution: Not pertinent

Heat of Polymerization: Not pertinent

Heat of Fusion: 19.18 cal/g

Limiting Value: Currently not available

REID Vapor Pressure: 52.4 psia

UN TDG, 2007

UN No.	Name and description	Class or division	Subsi-diary risk	UN packing group	Special provi-sions	Limited and excepted quantities		Packagings and IBCs		Portable tanks and bulk containers	
								Packing instruction	Special packing provisions	Instruc-tions	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
0487	SIGNALS, SMOKE†	1.3G				0	E0	P135			
0488	AMMUNITION, PRACTICE†	1.3G				0	E0	P130 LP101	PP67 L1		
0489	DINITROGLYCOLURIL (DINGU)†	1.1D				0	E0	P112(b) P112(c)			
0490	NITROTRIAZOLONE (NTO)†	1.1D				0	E0	P112(b) P112(c)			
0491	CHARGES, PROPELLING†	1.4C				0	E0	P143	PP76		
0492	SIGNALS, RAILWAY TRACK, EXPLOSIVE†	1.3G				0	E0	P135			
0493	SIGNALS, RAILWAY TRACK, EXPLOSIVE†	1.4G				0	E0	P135			
0494	JET PERFORATING GUNS, CHARGED, oil well, without detonator†	1.4D				0	E0	P101			
0495	PROPELLANT, LIQUID†	1.3C			224	0	E0	P115	PP53 PP54 PP57 PP58		
0496	OCTONAL	1.1D				0	E0	P112(b) P112(c)			
0497	PROPELLANT, LIQUID†	1.1C			224	0	E0	P115	PP53 PP54 PP57 PP58		
0498	PROPELLANT, SOLID†	1.1C				0	E0	P114(b)			
0499	PROPELLANT, SOLID†	1.3C				0	E0	P114(b)			
0500	DETONATOR ASSEMBLIES, NON-ELECTRIC for blasting†	1.4S				0	E0	P131			
0501	PROPELLANT, SOLID†	1.4C				0	E0	P114(b)			
0502	ROCKETS with inert head†	1.2C				0	E0	P130 LP101	PP67 L1		
0503	AIR BAG INFLATORS, or AIR BAG MODULES, or SEAT-BELT PRETENSIONERS†	1.4G			235 289	0	E0	P135			
0504	1H-TETRAZOLE	1.1D				0	E0	P112(c)	PP48		
0505	SIGNALS, DISTRESS, ship†	1.4G				0	E0	P135			
0506	SIGNALS, DISTRESS, ship†	1.4S				0	E0	P135			
0507	SIGNALS, SMOKE†	1.4S				0	E0	P135			
0508	1-HYDROXYBENZOTRIAZOLE, ANHYDROUS, dry or wetted with less than 20% water, by mass	1.3C				0	E0	P114(b)	PP48 PP50		
1001	ACETYLENE, DISSOLVED	2.1				0	E0	P200			
1002	AIR, COMPRESSED	2.2			292	120 ml	E1	P200			
1003	AIR, REFRIGERATED LIQUID	2.2	5.1			0	E0	P203		T75	TP5 TP22
1005	AMMONIA, ANHYDROUS	2.3	8		23	0	E0	P200		T50	
1006	ARGON, COMPRESSED	2.2				120 ml	E1	P200			
1008	BORON TRIFLUORIDE	2.3	8			0	E0	P200			
1009	BROMOTRIFLUOROMETHANE (REFRIGERANT GAS R 13B1)	2.2				120 ml	E1	P200		T50	
1010	BUTADIENES, STABILIZED or BUTADIENES AND HYDROCARBON MIXTURE, STABILIZED, containing more than 40% butadienes	2.1				0	E0	P200		T50	
1011	BUTANE	2.1				0	E0	P200		T50	
1012	BUTYLENE	2.1				0	E0	P200		T50	

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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).

4.2 Production and Use

Butane and isobutane are produced from raw natural gas and from petroleum streams by catalytic cracking, catalytic re-forming, and other refining processes. Liquid butane is recovered from the feedstock gas through a process involving refrigeration, adsorption, expansion, compression, fractionation, and other cryogenic steps (58). Butane is used in the production of ethylene and 1,3-butadiene; in the blending of gasoline or motor fuel; in the synthesis of high octane blend stocks of motor fuel; in the synthesis of acetic acid, maleic anhydride, isobutane, and other chemicals; as a constituent in liquefied natural gas and substitute natural gas; as a refrigerant and aerosol propellant; and as a solvent in the liquid–liquid extraction of heavy oils in deasphalting processes (58).

4.3 Exposure Assessment

4.3.1 Air

Butane has been measured in the atmosphere using gas chromatography and headspace techniques (38). A gas chromatography–mass spectrometric method has been described for the survey and determination of trace components in air, including butane (59). The determination of hydrocarbons, including butane, in the parts per billion range, is accomplished using glass capillary columns coated with aluminum oxide (25). In addition, colorimetric detection tubes, permeation tubes, and direct reading gas analyzers have been employed to quantitate the levels of butane in the air (26).

4.3.2 Background Levels: NA

4.3.3 Workplace Methods: NA

4.3.4 Community Methods: NA

4.3.5 Biomonitoring/Biomarkers

Detection and quantification of butane in tissues of rats and mice, such as brain, liver, kidney, spleen, and perinephric fat, have been conducted by gas chromatography methods (54).

4.4 Toxic Effects

4.4.1 Experimental Studies

4.4.1.1 Acute Toxicity. The 4-h lethal concentration 50% kill (LC_{50}) for the rat is 658 mg/L, and the 2-h LC_{50} for the mouse is 680 mg/L (54). Butane is anesthetic to mice at 13% in 25 min and at 22% in 1 min. Respiratory exposure to mice to 27% for 2 h caused death in 40% of the animals and 31% caused 60% mortality (60). In dogs, lethality was observed at concentrations of 20 to 25%; anesthesia and relaxation preceded death (60). There was only a small margin of safety between anesthetic and lethal concentrations. Mixing butane and isobutylene has an additive CNS depressant effect in rats (61).

The mechanism concerning the anesthetic properties of butane is similar to that of ethane and propane.

4.4.1.2 Chronic and Subchronic Toxicity: NA

4.4.1.3 Pharmacokinetics, Metabolism, and Mechanisms. Butane is partially absorbed in the rat lung and is translocated to the brain, kidney, liver, spleen, and perinephric fat (54). In both rats and mice the brain levels of butane correlated with the degree of CNS depression and narcosis (54). Hydroxylation of butane occurs in rat liver microsomes to produce 2-butanol as the major metabolite (30). Butane is the lowest molecular weight alkane demonstrated to substrate-bind with cytochrome P450. If 2-butanol is the major metabolite formed in animals, it would be expected to be eliminated in expired air (62). 2-Butanol may also be conjugated with glucuronic acid or be oxidized to methyl ethyl ketone, which, in turn, is expired (63). Because of its volatile nature, elimination of butane by exhalation can be anticipated (58). Its elimination half-life is 0.13 h at nonsaturating concentrations (24).

4.4.1.4 Reproductive and Developmental: NA

4.4.1.5 Carcinogenesis: NA

4.4.1.6 Genetic and Related Cellular Effects Studies. The mutagenic potential of butane was evaluated *in vitro* at several concentrations using the Ames *Salmonella typhimurium* microsome assay. Butane was not mutagenic (64). Butane was negative in *Drosophila melanogaster* sex-linked recessive lethal/reciprocal translocation tests (33).

4.4.1.7 Other: Neurological, Pulmonary, Skin Sensitization, etc. Butane is a weak cardiac sensitizer in the dog (65). Concentrations of 5000 ppm in the anesthetized dog may cause hemodynamic changes, such as decreases in cardiac output, left ventricular pressure and stroke volume, myocardial contractility, and aortic pressure (42). Butane does not cause respiratory or eye irritation in rabbits, and it appears to be mildly to moderately irritating to the rabbit skin (46).

4.4.2 Human Experience

4.4.2.1 General Information. On direct contact, liquefied butane may cause burns or frostbite to the eyes, skin, or mucous membranes. The inhalation of 10,000 ppm for 10 min may result in CNS depression but produces no systemic effects (50). It can cause blurred vision and can be aspirated resulting in pneumonitis.

4.4.2.2 Clinical Cases

4.4.2.2.1 Acute Toxicity. A 2-year old girl developed seizures, hypotension, and recurrent ventricular tachycardia after unintentional exposure to a spray can containing butane, isobutane, and propane (66).

4.4.2.2.2 Chronic and Subchronic Toxicity. A 16-year old girl used butane as an abuse drug. She inhaled it for a year, and during the 3 months prior to the report, she inhaled about 22 canisters (232 mL). She used the cover of the canister as the mask for the abuse. She suffered from visual hallucinations during initial abuse and became increasingly irritable. Gradual deterioration in social functioning led to social isolation with very little contact with her peer group. Physical examination was unremarkable (67).

4.5 Standards, Regulations, or Guidelines of Exposure

Butane is on the EPA TSCA Chemical Inventory and the Test Submission Data Base (16). Table 49.4 shows the occupational exposure limits for butane in the United States, and the international limits are shown in Table 49.5.

Table 49.4. Occupational Exposure Limits for Butane in the United States[a]

Exposure Limits	OSHA PEL	NIOSH Recommended Exposure Limit	ACGIH TLV
Time-weighted average	—	800 ppm (1900 mg/m^3)	800 ppm (1900 mg/m^3)
Short-term exposure limit	—	—	—
Ceiling limit	—	—	—

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

Table 49.5. Occupational Exposure Limits for Butane in Different Countries[a]

Country	Exposure limit
Australia	TWA 800 ppm (1900 mg/m^3)
Austria	TWA 1000 ppm (2300 mg/m^3)
Belgium	TWA 800 ppm (1900 mg/m^3)
Denmark	TWA 500 ppm (1200 mg/m^3)
Finland	TWA 800 ppm (1900 mg/m^3); STEL 1000 ppm (2350 mg/m^3)
France	TWA 800 ppm (1900 mg/m^3)
Germany	TWA 1000 ppm (2350 mg/m^3)
Hungary	TWA 300 ppm; STEL 900 ppm
India	TWA 800 ppm (1900 mg/m^3)
Ireland	TWA 600 ppm (1430 mg/m^3); STEL 750 ppm (1780 mg/m^3)
Japan	TWA 500 ppm (1200 mg/m^3)
Mexico	TWA 800 ppm (1900 mg/m^3)
The Netherlands	TWA 600 ppm (1430 mg/m^3)
Poland	TWA 1900 mg/m^3; STEL 3000 mg/m^3
Russia	TWA 500 ppm; STEL 300 ppm
Switzerland	TWA 800 ppm (1900 mg/m^3)
United Kingdom	TWA 600 ppm (1450 mg/m^3); STEL 750 ppm (1810 mg/m^3)

[a]From Refs. 19 and 20.

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

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heated to decomposition it emits very toxic fumes of Br^- and NO_x. See also BARBITURATES and ALLYL COMPOUNDS.

BOR250 CAS: 3486-86-0 HR: 3
BUTALLYLONAL SODIUM
mf: $C_{11}H_{14}BrN_2O_3{\cdot}Na$ mw: 325.17
PROP: Powder. Sol in H_2O and EtOH.
SYNS: sec-BUTYL-BROM-ALLYL BARBITURIC ACID SODIUM SALT ◻ SODIUM-5-(2-BROMOALLYL)-5-sec-BUTYLBARBITURATE
TOXICITY DATA with REFERENCE:
orl-cat LD50:135 mg/kg JPETAB 88,260,46
orl-rbt LD50:375 mg/kg JPETAB 42,253,31
ipr-rbt LD50:75 mg/kg JPETAB 42,253,31
SAFETY PROFILE: Poison by ingestion and intraperitoneal routes. When heated to decomposition it emits very toxic fumes of Br^- and NO_x. See also BARBITURATES.

BOR350 CAS: 18109-81-4 HR: 2
BUTAMIRATE CITRATE
mf: $C_{18}H_{29}NO_3{\cdot}C_6H_8O_7$ mw: 499.62
PROP: Crystals from Me_2CO. Mp: 75°.
SYNS: ABBOTT 36581 ◻ ACODEEN ◻ BUTAMYRATE CITRATE ◻ 2-((2-(DIETHYLAMINO)ETHOXY)ETHYL-2-PHENYLBUTYRATE CITRATE ◻ α-ETHYLBENZENEACETIC ACID-2-((2-DIETHYL AMINO)ETHOXY)ETHYL ESTER CITRATE ◻ HH-197 ◻ PHENYL ACETIC ACID DIETHYLAMINOETHOXY-ETHANOL ESTER CITRATE ◻ 2-PHENYLBUTYRIC ACID 2-(2-DIETHYLAMINO) ETHOXY)ETHYL ESTER CITRATE ◻ SINCODEEN ◻ SINCODEX ◻ SINCODIN ◻ SINCODIX ◻ SINECOD
TOXICITY DATA with REFERENCE:
orl-rat LD50:4164 mg/kg TOIZAG 18,115,71
scu-rat LD50:3638 mg/kg TOIZAG 18,115,71
orl-mus LD50:865 mg/kg TOIZAG 18,115,71
SAFETY PROFILE: Moderately toxic by ingestion and subcutaneous routes. Experimental reproductive effects. An experimental teratogen. When heated to decomposition it emits toxic fumes of NO_x. See also ESTERS.

BOR500 CAS: 106-97-8 HR: 3
BUTANE
DOT: UN 1011
mf: C_4H_{10} mw: 58.14
PROP: Colorless gas; faint disagreeable odor. Bp: −0.5°, fp: −135°, lel: 1.9%, uel: 8.5%, flash p: −76°F (CC), d: 0.599, autoign temp: 761°F, vap press: 2 atm @ 18.8°, vap d: 2.046. Sldly sol in H_2O; mod sol in Et_2O and $CHCl_3$.
SYNS: n-BUTANE (DOT) ◻ BUTANE MIXTURES (DOT) ◻ BUTANEN (DUTCH) ◻ BUTANI (ITALIAN) ◻ DIETHYL ◻ METHYLETHYLMETHANE
TOXICITY DATA with REFERENCE:
ihl-rat LC50:658 g/m³/4H FATOAO 30,102,67
ihl-mus LC50:680 g/m³/2H FATOAO 30,102,67
CONSENSUS REPORTS: Reported in EPA TSCA Inventory.
OSHA PEL: TWA 800 ppm
ACGIH TLV: TWA 800 ppm
DFG MAK: 1000 ppm (2400 mg/m³)
DOT CLASSIFICATION: 2.1; Label: Flammable Gas
SAFETY PROFILE: Mildly toxic by inhalation. Causes drowsiness. An asphyxiant. Very dangerous fire hazard when exposed to heat, flame, or oxidizers. Highly explosive when exposed to flame, or when mixed with [$Ni(CO)_4 + O_2$]. To fight fire, stop flow of gas. When heated to decomposition it emits acrid smoke and fumes.

BOR750 CAS: 590-88-5 HR: 3
1,3-BUTANEDIAMINE
mf: $C_4H_{12}N_2$ mw: 88.18
PROP: Liquid. Bp: 142–150°, flash p: 125°F, d: 0.85, vap d: 3.04.
SYN: 1,3-DIAMINOBUTANE
TOXICITY DATA with REFERENCE:
skn-rbt 10 mg/24H open SEV AMIHBC 4,119,51
eye-rbt 250 µg open SEV AMIHBC 4,119,51
orl-rat LD50:1350 mg/kg AMIHBC 4,119,51
skn-rbt LD50:430 mg/kg AMIHBC 4,119,51
SAFETY PROFILE: Moderately toxic by ingestion and skin contact. Severe skin and eye irritant. Flammable liquid when exposed to heat or flame. To fight fire, use alcohol foam, foam, CO_2, dry chemical. Incompatible with oxidizing materials. When heated to decomposition it emits toxic fumes of NO_x. See also 1,4-BUTANEDIAMINE and AMINES.

BOS000 CAS: 110-60-1 HR: 3
1,4-BUTANEDIAMINE
mf: $C_4H_{12}N_2$ mw: 88.18
PROP: Crystals with strong odor. Mp: 27–28°, bp: 158–159°.
SYNS: BUTYLENEDIAMINE ◻ 1,4-BUTYLENEDIAMINE ◻ 1,4-DIAMINOBUTANE ◻ PUTRESCIN ◻ PUTRESCINE ◻ TETRAMETHYLENEDIAMINE ◻ 1,4-TETRAMETHYLENE DIAMINE
TOXICITY DATA with REFERENCE:
cyt-hmn:hla 2 mmol/L JCLLAX 78,217,71
dns-mus:lvr 2 mmol/L AMOKAG 33,149,79
dni-mus:ast 10 mmol/L AMOKAG 33,149,79
dni-mus:lvr 20 mmol/L AMOKAG 33,149,79
orl-mus LDLo:1600 mg/kg AECTCV 14,111,85
orl-rbt LDLo:1600 mg/kg CRSBAW 83,481,20
orl-rbt LDLo:1600 mg/kg CRSBAW 83,481,20
scu-rbt LDLo:1 g/kg ZEPTAT 17,59,15
ivn-rbt LDLo:80 mg/kg CRSBAW 83,481,20
rec-rbt LDLo:400 mg/kg CRSBAW 83,481,20
CONSENSUS REPORTS: Reported in EPA TSCA Inventory.
SAFETY PROFILE: Poison by subcutaneous, intravenous, and rectal routes. Moderately toxic by ingestion. An experimental teratogen. Human mutation data reported. When heated to decomposition it emits toxic fumes of NO_x. See also 1,3-BUTANEDIAMINE and AMINES.

BOS050 CAS: 119422-08-1 HR: 3
1,4-BUTANEDIAMINE, N,N'-BIS(4-(ETHYL-AMINO) BUTYL)-
mf: $C_{16}H_{38}N_4$ mw: 286.58

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
Brazil Wax	See Carnauba Wax.												
Bromobenzene C_6H_5Br (Phenyl Bromide) 108-86-1	II	124 (51)	1049 (565)			1.5	5.4	313 (156)	No	3	1	2	0
1-Bromobutane	See Butyl Bromide.												
4-Bromodiphenyl $C_6H_5C_6H_4Br$ 92-66-0	IIIB	291 (144)						592 (311)	No	2	1	1	0
Bromoethane	See Ethyl Bromide.												
Bromomethane	See Methyl Bromide.												
1-Bromopentane	See Amyl Bromide.												
3-Bromopropene	See Allyl Bromide.												
3-Bromopropyne $HC{:}CCH_2Br$ (Propargyl Bromide) 106-96-7	IB	50 (10)	615 (324)	3.0		1.57	4.10	192 (89)	No	4	3	3	4
	See NFPA 49 contained in this guide.												
o-Bromotoluene $BrC_6H_4CH_3$ 95-46-5	IIIA	174 (79)				1.4	5.9	359 (182)	No	3	1	2	0
p-Bromotoluene $BrC_6H_4CH_3$ 106-38-7	IIIA	186 (86)				1.4	5.9	383 (184)	No	3	2	2	0
1,3-Butadiene $CH_2{:}CHCH{:}CH_2$ (Erythrene) 106-99-0		Gas	788 (420)	2.0	12.0		1.9	24 (−4)	No	8	2	4	2
	Note: Polymerizes. See NFPA 49 contained in this guide.												
Butadiene Monoxide $CH_2{:}CHCHOCH_2$ (Vinylethylene Oxide) 930-22-3	IB	<−58 (<−50)				0.9	2.4	151 (66)		1		3	2
Butanal	See Butyraldehyde.												
Butanal Oxime	See Butyraldoxime.												
Butane $CH_3CH_2CH_2CH_3$ 106-97-8	IA	Gas [−76 (−80)]	550 (287)	1.9	8.5		2.0	31 (−1)	No	6	1	4	0
1,3-Butanediamine $NH_2CH_2CH_2CHNH_2CH_3$ (1,3-Diaminobutane) 590-88-5		125 (52) (oc)				0.9	3.0	289–302 (143–150)	Yes	5	3	2	0
1,2-Butanediol $CH_3CH_2CHOHCH_2OH$ (1,2-Dihydroxybutane) (Ethylethylene Glycol) 584-03-2	II	104 (40)				1.0	3.1	381 (194)	Slight	5	1	2	0
1,3-Butanediol	See β-Butylene Glycol.												
1,4-Butanediol $HOCH_2CH_2CH_2CH_2OH$ (Tetramethylene Glycol) 110-63-4		250 (121) (oc)	662 (350)	1.95	18.3	1.0+	3.1	442 (228)	Yes	2 6	1	1	0
	Note: Melting point 64–66 (18–19).												
2,3-Butanediol $CH_3CHOHCHOHCH_3$ 513-85-9		185 (85)	756 (402)			1.0+		363 (184)	Yes	5	1	1	0
	Note: Melting point 77 (25).												
2,3-Butanedione $CH_3COCOCH_3$ (Diacetyl) 431-03-8	IC	80 (27)				1.0−	3.0	190 (88)	Yes	5 1	2	3	0

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
1381	1-Bromo-4-vinylbenzene		C_8H_7Br	2039-82-9	183.046		7.7	212; 103[20]	1.3904[20]	1.5947[20]	i H_2O; vs chl; s HOAc
1382	Bromphenilamine		$C_{16}H_{19}BrN_2$	86-22-6	319.239	ye oily liq		150[0.5]			s dil acid
1383	Brucine		$C_{23}H_{26}N_2O_4$	357-57-3	394.463	mcl pr (w +4)	178				sl H_2O; eth, bz; vs EtOH, chl
1384	Brucine hydrochloride	2,3-Dimethoxystrychnidin-10-one, monohydrochloride	$C_{23}H_{27}ClN_2O_4$	5786-96-9	430.924	pr					vs H_2O, EtOH
1385	Brucine sulfate heptahydrate	2,3-Dimethoxystrychnidin-10-one, sulfate, heptahydrate	$C_{46}H_{66}N_4O_{19}S$	60583-39-3	1013.113	nd (w)					s H_2O; sl EtOH; chl; tfa; vs MeOH; i bz
1386	Bucloloma	5-Butyl-1-cyclohexyl-2,4,6(1*H*,3*H*,5*H*)-pyrimidinethione	$C_{14}H_{24}N_2O_3$	841-73-6	266.336	nd (MeOH)	84	186[10]			
1387	Bulobalin		$C_{28}H_{36}O_6$	471-95-4	444.560	cry (+1 al)	223 dec				i H_2O; s EtOH; chl
1388	Bulbocapnine		$C_{19}H_{19}NO_4$	298-45-3	325.359	pr (al)	199.5				i H_2O; s EtOH; vs chl
1389	sec-Bumeton	*N*-sec-Butyl-*N*'-ethyl-6-methoxy-1,3,5-triazine-2,4-diamine	$C_{10}H_{18}N_6O$	26259-45-6	226.281		87				
1390	BUSAN 72A	(2-Benzothiazolylthio)methyl thiocyanate	$C_9H_6N_2S_3$	21564-17-0	238.352	liq		dec			
1391	Butachlor		$C_{17}H_{26}ClNO_2$	23184-66-9	311.847		<-5	156[5]	1.070[25]		
1392	1,2-Butadiene	Methylallene	C_4H_6	590-19-2	54.091	vol liq or gas	-136.2	10.9	0.678[0]	1.4208[1]	i H_2O; msc EtOH, eth; vs bz
1393	1,3-Butadiene	Divinyl	C_4H_6	106-99-0	54.091	col gas	-108.91	-4.41	0.6149[25] (p>1 atm)	1.4292[-25]	i H_2O; s EtOH, eth, bz; vs aca
1394	1,3-Butadien-1-ol acetate		$C_6H_8O_2$	1515-76-0	112.127			58[40]	0.945[25]	1.4690[20]	
1395	(*trans*)-1,3-Butadienylbenzene		$C_{10}H_{10}$	16939-57-4	130.186		2.3	76[11]	0.9266[20]	1.5089[20]	i H_2O; s EtOH, eth, aca, bz
1396	1,3-Butadiyne	Diacetylene	C_4H_2	460-12-8	50.059	vol liq or gas	-36.4	10.3	0.7364[0]	1.4189[-5]	vs H_2O, eth, acet; s chl, EtOH
1397	Bualbital	5-Isobutyl-5-allyl-2,4,6(1*H*,3*H*,5*H*)-pyrimidinetrione	$C_{11}H_{16}N_2O_3$	77-26-9	224.256	pr	138.5				sl H_2O; s EtOH, eth, aca, chl; i lig
1398	Butanal	Butyraldehyde	C_4H_8O	123-72-8	72.106	liq	-96.86	74.8	0.8016[20]	1.3843[20]	s H_2O; msc EtOH; vs acs, bz; sl chl
1399	Butanal oxime		C_4H_9NO	110-69-0	87.120	liq	-29.5	154	0.922[20]		vs H_2O, aca, bz; msc EtOH, eth; s chl
1400	Butanamide	Butyramide	C_4H_9NO	541-35-5	87.120	ll (bz)	114.8	216	0.8650[105]	1.4087[130]	sl H_2O, eth; i bz; s EtOH
1401	Butane		C_4H_{10}	106-97-8	58.122	col gas	-138.3	-0.5	0.573[25] (p>1 atm)	1.3326[20]	i H_2O; vs EtOH, eth, chl
1402	Butanedial		$C_4H_6O_2$	638-37-9	86.090			dec 170; 59[9]	1.065[20]	1.4262[19]	vs H_2O, aca; ath; EtOH
1403	1,4-Butanediamine	Putrescine	$C_4H_{12}N_2$	110-60-1	88.151	ll	21.91	158.5	0.877[25]	1.4969[20]	s H_2O
1404	1,4-Butanediamine dihydrochloride		$C_4H_{14}Cl_2N_2$	333-93-7	161.073	nd or ll (al, w)	280 dec	sub			vs H_2O, EtOH; i eth, bz, MeOH
1405	1,2-Butanediol, (±)		$C_4H_{10}O_2$	26171-83-5	90.121			190.5	1.0024[20]	1.4378[20]	s H_2O, EtOH; aca
1406	1,3-Butanediol	1,3-Butylene glycol	$C_4H_{10}O_2$	107-88-0	90.121		<-50	207.5	1.0053[20]	1.4401[20]	
1407	1,4-Butanediol	Tetramethylene glycol	$C_4H_{10}O_2$	110-63-4	90.121		20.4	235	1.0171[20]	1.4468[20]	msc H_2O; s EtOH. DMSO; sl eth
1408	2,3-Butanediol		$C_4H_{10}O_2$	6982-25-8	90.121	cry (eth)	7.6	182.5	1.0033[20]	1.4310[25]	msc H_2O, EtOH; s eth, ace, chl
1409	1,4-Butanediol diacetate		$C_8H_{14}O_4$	628-67-1	174.195		12	229	1.0479[15]	1.4251[15]	
1410	1,4-Butanediol diacrylate		$C_{10}H_{14}O_4$	1070-70-8	198.216			83[0.3]	1.105[23]		
1411	1,4-Butanediol diglycidyl ether	1,4-Bis(2,3-epoxypropoxy)butane	$C_{10}H_{18}O_4$	2425-79-8	202.248			266; 155[11]	1.15	1.4611[30]	
1412	1,3-Butanediol dimethacrylate		$C_{12}H_{18}O_4$	1189-08-8	226.269			290		1.4496[25]	vs ace, eth, EtOH, lig
1413	1,4-Butanediol dimethacrylate		$C_{12}H_{18}O_4$	2082-81-7	226.269	liq		133[1], 76[0.007]	1.025[20]	1.4560[20]	sl H_2O
1414	1,4-Butanediol dimethylsulfonate	Busulfan	$C_6H_{14}O_6S_2$	55-98-1	246.301	cry	116				i H_2O; sl EtOH; ace
1415	2,3-Butanedione	Diacetyl	$C_4H_6O_2$	431-03-8	86.090	liq	-1.2	88	0.9808[16]	1.3951[20]	vs H_2O; msc EtOH; eth; s bz, cic
1416	2,3-Butanedione monooxime		$C_4H_7NO_2$	57-71-6	101.105	pr (chl), ll (w)	76.8	185.5			sl H_2O; vs EtOH, eth, chl; s alk
1417	Butanedioyl dichloride	Succinyl chloride	$C_4H_4Cl_2O_2$	543-20-4	154.980	pl or ll	20	193.3	1.374[20]	1.4633[20]	s eth, ace, bz
1418	1,4-Butanedithiol	Tetramethylenedithiol	$C_4H_{10}S_2$	1191-08-8	122.252	liq	-53.9	195.5	1.0021[0]	1.5250[20]	i H_2O; vs EtOH; sl cic

...l; from petroleum gases, ...
...e or butene-butane mixtures
...anuf: *Faith, Keyes & Clark's*
...m, M. K. Moran, Eds. (Wi...
...) pp 164-172. Toxicity stud...
...ol. 26, 69 (1944). *Review*...
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...y, "Butadiene" in *Vinyl and*...
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pt −108.902°. Densities ...
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in 1 atm): 2 atm: 15.3°; 5 atm...
4.0°; 30 atm: 139.8°; 40 atm...
.8°; critical pressure 42.6 a...
pid. 422. Stability: *Ind. ...*
with *o*-dihydroxybenzene: ...
US 2373754. Explosion limi...
5. Polymerizes and copolym...
ce of sodium, thereby formi...
ble in water; slightly soluble...
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If overexposure are irritation...
lightheadedness; teratogenic...
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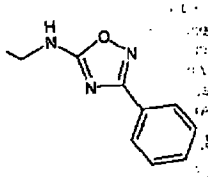
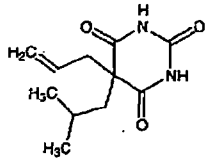
...-35-7] *NN*-Dibutyl-*N'*-(3-...
...iediamine; 5-[[2-(dibutylam...
...diazole; 3-phenyl-5-(dibutyl...
$C_{18}H_{28}N_4O$; mol wt 316...
...06%. Prepn: FR M3334 (...
65, 1967 to Aron-Samuel); ...
J. Sterne *et al.*, *Therapie* 2...
...ontaine, R. Fontaine, *ibid.* 2...



...] LA-1221; Adrevil; Hem...
...HCl; mol wt 352.90. mp ...
2500 s.c., 625 orally; LD_{50} ...
(Sterne).
...ipheral).

...-9] 5-(2-Methylpropyl)-5-...
...nidinetrione; 5-allyl-5-(...
...hylpropyl)barbituric acid; ...

Butalbital. [77-26-9] 5-Allyl-5-isobutylbarbituric acid; alisobumal; allylbarbital; isobarbital; tetralbital; Sandoptal. $C_{11}H_{16}N_2O_3$; mol wt 224.26. C 58.91%, H 7.19%, N 12.49%, O 21.40%. Prepn: Volwiler, *J. Am. Chem. Soc.* 47, 2236 (1925).

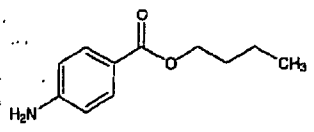


Prisms, mp 138-139°. Slightly bitter taste. Practically insol in water and petr ether. Sol in alcohol, chloroform, ether, acetone, glacial acetic acid, also in solns of fixed alkali hydroxides. A satd aq soln is acid to litmus.

Note: This is a controlled substance (depressant): **21 CFR**, 1308.13.

THERAP CAT: Sedative, hypnotic.

1512. Butamben. [94-25-7] 4-Aminobenzoic acid butyl ester; butyl aminobenzoate; *n*-butyl *p*-aminobenzoate; Butesin; Butoform; Planoform; Scuroforme. $C_{11}H_{15}NO_2$; mol wt 193.24. C 68.37%, H 7.82%, N 7.25%, O 16.56%. Prepn: Brill, *J. Am. Chem. Soc.* 43, 1322 (1921); Adams, Volwiler, **US 1440652** (1923 to Abbott); **GB 252870**; *C.A.* 17, 1243 (1923); *C.A.* 21, 2478 (1927).

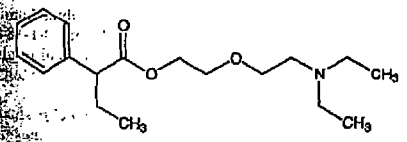


Crystals from alc, mp 57-59°. bp_6 174°. One gram dissolves in about 7 liters of water. Sol in dil acids, alcohol, chloroform, ether, and fatty oils. It is hydrolyzed slowly when boiled with water.

THERAP CAT: Anesthetic (local).

THERAP CAT (VET): Anesthetic (local).

1513. Butamirate. [18109-80-3] α-Ethylbenzeneacetic acid 2-[2-(diethylamino)ethoxy]ethyl ester; 2-phenylbutyric acid 2-[2-(diethylamino)ethoxy]ethyl ester; 2-[2-(diethylamino)ethoxy]ethyl α-phenylbutyrate; butamyrate. $C_{18}H_{29}NO_3$; mol wt 307.43. C 70.32%, H 9.51%, N 4.56%, O 15.61%. Prepd by the esterification of α-phenylethylacetyl chloride with diethylaminoethoxyethanol: DE 1115815; Houssier, **US 3349114** (1963, 1967, both to Hommel Co).

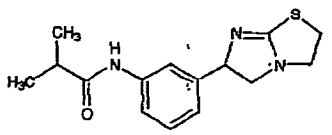


Practically colorless liquid with peculiar odor. bp_1 140-155°. Practically insol in water. Very sol in alcohol, acetone, ether.

Citrate [18109-81-4] Abbott 36581; HH-197; Acodeen; Pantussicodix; Sinecod. $C_{18}H_{29}NO_3.C_6H_8O_7$; mol wt 499.55. Hygroscopic crystals from acetone, mp 75°.

THERAP CAT: Antitussive.

1514. Butamisole. [54400-59-8] 2-Methyl-*N*-[3-(2,3,5,6-tetrahydroimidazo[2,1-*b*]thiazol-6-yl)phenyl]propanamide; (−)-2-[3-(2,3,5,6-tetrahydroimidazo[2,1-*b*]thiazol-6-yl)propionamido]-4-phenylthiazole. $C_{19}H_{19}N_3OS$; mol wt 289.40. C 62.25%, H 6.62%, N 14.53%, O 5.53%, S 11.08%. Prepn: L. D. Spicer, J. J. Hand, ZA 6802503 (1972 to Am. Cyanamid), *C.A.* 78, 72151h (1973). Prepn and resolution of isomers: *eidem*, FR 2199979; *eidem*, **US 3899583** (1975 both to Am. Cyanamid). Efficacy and safety in dogs: Clifford *et al.*, *Vet. Med. Small Anim. Clin.* 74, 487 (1979). Evaluation in horses and ponies: R. B. Grieve *et al.*, *Am. J. Vet. Res.* 39, 1 (1979).



Hydrochloride. [54400-62-3] CL-206214; Styquin. $C_{15}H_{19}N_3OS.HCl$; mol wt 325.86.

THERAP CAT (VET): Anthelmintic.

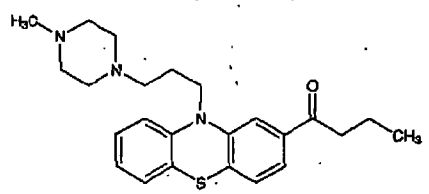
1515. Butane. [106-97-8] *n*-Butane. C_4H_{10}; mol wt 58.12. C 82.66%, H 17.34%. $CH_3CH_2CH_2CH_3$. Occurrence: in petroleum, Mabery, *J. Am. Chem. Soc.* 30, 143 (1908); in natural gas and in refinery cracking products. Prepd from C_2H_5I and sodium amalgam: Löwig, *Jahresber. Fortschr. Chem.* 1860, 397, *Beilstein* vol. 1, 118. Recovery of butanes from natural and refinery gases: Kirkbride, Bertelli, *Ind. Eng. Chem.* 35, 1242 (1943); Walters, *ibid.* 47, 2544 (1955); Gilmore, Bauer, *Oil Gas J.* 50, 84, 90, 94, 119 (1951), *C.A.* 46, 1743d (1952). Separation of butane and isobutane: Stone, *Pet. Refin.* 25(4), 164 (1946), *C.A.* 43, 2414 (1949). Handbook: *Butane-Propane Gases*, L. C. Denny *et al.*, Eds. (Chilton Co., Los Angeles, 4th ed., 1962) 383 pp.

Flammable gas. bp −0.50°. d(gas) 2.046 (air = 1). One vol of water dissolves 0.15 vol and 1 vol of alcohol 18 vols of the gas at 17° and 770 mm; 1 vol of ether or chloroform at 17° dissolves 25 or 30 vols of the gas, resp.

Caution: Potential symptoms of overexposure are drowsiness, narcosis, asphyxia; direct contact with liquid may cause frostbite. *See NIOSH Pocket Guide to Chemical Hazards* (DHHS/NIOSH 97-140, 1997) p 34.

USE: As producer gas; raw material for motor fuels, in the manuf of synthetic rubbers.

1516. Butaperazine. [653-03-2] 1-[10-[3-(4-Methyl-1-piperazinyl)propyl]-10*H*-phenothiazin-2-yl]-1-butanone; 2-butyryl-10-[3-(4-methyl-1-piperazinyl)propyl]phenothiazine; *N*-[γ-(4'-methyl-1'-piperazinyl)propyl]-3-butyrylphenothiazine; butyrylperazine; Bayer 1362; Repoise; Tyrylen. $C_{24}H_{31}N_3OS$; mol wt 409.59. C 70.38%, H 7.63%, N 10.26%, O 3.91%, S 7.83%. Prepn: Hoerlein *et al.*, **DE 1120451** (1961 to Bayer), *C.A.* 57, 4677c (1962).



$bp_{0.05}$ 270-280°.

Dimaleate. [1063-55-4] Randolectil. $C_{24}H_{31}N_3OS.2C_4H_4O_4$; mol wt 641.73.

Maleate. $C_{24}H_{31}N_3OS.C_4H_4O_4$. Crystals from carbon tetrachloride, mp 180-182°.

THERAP CAT: Antipsychotic.

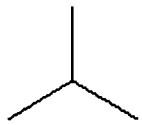
1517. Butedronic Acid. [51395-42-7] (Diphosphonomethyl)butanedioic acid; (diphosphonomethyl)succinic acid; 2,3-dicarboxypropane-1,1-diphosphonic acid; DPD. $C_5H_{10}O_{10}P_2$; mol wt 292.07. C 20.56%, H 3.45%, O 54.78%, P 21.21%. Prepn: A. Heins *et al.*, **DE 2217692** (1973 to Henkel); *eidem*, **US 3923876** (1975 to Bayer A.G.); K. H. Worms, H. Blum, *Z. Anorg. Allg. Chem.* 457, 219 (1979); and physical-chemical properties: N. Vanlic-Razumenic *et al.*, *J. Serb. Chem. Soc.* 51, 63 (1986). Clinical pharmacokinetics of ^{99m}Tc complex: C. Schümichen, H. Schmidt, *Nuklearmedizin Suppl.* 19, 930 (1982). Clinical evaluation of ^{99m}Tc complex as skeletal imaging agent: G. Godart *et al.*, *Clin. Nucl. Med.* 11, 92 (1986).

Merck, 2006

資料IB-1(CD)

Isobutane

- 2-Methylpropane

Formula	C_4H_{10}
Structure	
Description	Isobutane is a colorless gas with a faint petroleum-like odor.
Uses	Chemical intermediate for alkylate gasoline, component to control volatility of gasoline, chemical intermediate for propylene oxide, tert-butyl alcohol.

Registry Numbers and Inventories.

CAS	75-28-5
EC (EINECS/ELINCS)	200-857-2
EC Index Number	601-004-01-8
EC Class	Extremely flammable; Carcinogenic Category 1; Mutagenic Category 2
RTECS	TZ4300000
RTECS class	Other
UN (DOT)	1969
Beilstein/Gmelin	1730720
Beilstein Reference	4-01-00-00282
EPA OPP	97101
Swiss Giftliste 1	G-1699
Canada DSL/NDSL	DSL
US TSCA	Listed
Austrailia AICS	Listed
New Zealand	Listed
Japan ENCS (MITI)	Listed
Korea ECL	Listed

Properties.

Formula	C4H10
Formula mass	58.14
Melting point, °C	-255.3
Boiling point, °C	-11.7

Vapor pressure, mm_{Hg}	2580 (25 C)
Vapor density (air=1)	1
Critical temperature	134.69
Critical pressure	35.82
Density	0.559 g/cm3 (20 C)
Solubility in water	Slightly soluble
Viscosity	0.238 cp @ -10C
Surface tension	14.1 g/s2 @ -10 C
Refractive index	1.3518 (-25C)
Partition coefficient, pK_{ow}	2.76
Heat of fusion	2.57 kJ/mol
Heat of vaporization	21.3 kJ/mol
Heat of combustion	-3061 kJ/mol

Hazards and Protection.

Storage	Handle in accordance with all current regulations and standards. Subject to storage regulations: U.S. OSHA 29 CFR 1910.101. Grounding and bonding required.
WHMIS	A B1
Handling	Containers of this material may be hazardous when emptied. Since emptied containers retain product residues (vapor, liquid, and/or solid), all hazard precautions given in the data sheet must be observed.
Protection	Wear appropriate protective gloves, clothing and goggles. Always wear thermal protective clothing when handling refrigerated/cryogenic liquids.
Respirators	Wear positive pressure self-contained breathing apparatus (SCBA).
Small spills/leaks	Keep sparks, flames, and other sources of ignition away. Keep material out of water sources and sewers. Attempt to stop leak if without undue personnel hazard. Use water spray to knock-down vapors.
Stability	Stable.
Incompatibilities	Incompatible with the following: Strong oxidizers (e.g., nitrates & perchlorates), chlorine, fluorine, (nickel carbonyl + oxygen).
Decomposition	The gas mixes well with air, explosive mixtures are easily formed. Toxic fumes are formed when this material is heated.

Fire.

Flash Point,°C	-107
Autoignition, °C	460
Upper exp. limit, %	8.4
Lower exp. limit, %	1.8
Fire fighting	Do not extinguish fire unless flow can be stopped. Use water in flooding quantities as fog. Cool all affected containers with flooding quantities of water. Apply water from as far a distance as possible.
Fire potential	EXTREMELY FLAMMABLE.
Hazards	Vapors from liquefied gas are initially heavier than air and spread along ground. Vapors may travel to source of ignition and flash back. Containers may explode when heated. Ruptured cylinders may rocket.
NFPA Health	0
Flammability	4
Reactivity	0

Health.

Exposure limit(s)	MAK: 1000 ppm; 2350 mg/m3 (STEL); IV (MAK 1991) NIOSH REL: TWA 800 ppm (1900 mg/m3)
Poison_Class	-
Exposure effects	Rapid breathing and rapid heart rate are common. In severe cases abnormally low blood pressure, apnea, and cardiac arrest develop. Various disturbances including headache, dizziness, mood disturbances, numbness of the extremities, sleepiness, mental confusion, poor judgement and coordination, and memory loss may occur. Prolonged or severe hypoxia results in unconsciousness. Prolonged asphyxia may produce CNS injury. Hemiparesis has been reported with volatile substance abuse. Cerebral edema with brainstem herniation may occur. Seizures have been reported following intentional inhalation.
Ingestion	Nausea, vomiting, and gastrointestinal hemorrhage may develop.
Inhalation	Hyperventilation may develop.
Skin	Dermal exposure may cause frostbite injury. Severe tissue burns have been reported.
Eyes	Decreases in night vision, visual acuity, and visual fields (tunnel vision) may occur. Frothy mucous may be seen.

First aid

Ingestion	Seek medical assistance.
	Administer 100% humidified supplemental oxygen with assisted

Inhalation	ventilation as required. If hypoxia has been severe or prolonged, carefully evaluate for neurologic sequelae and provide supportive treatment as indicated.
Skin	Rewarming and a variety of topical treatments are indicated for frostbite injury. See main section for more information.
Eyes	Irrigate exposed eyes with copious amounts of tepid water for at least 15 minutes. If irritation, pain, swelling, lacrimation, or photophobia persist, the patient should be seen in a health care facility.

Transport.

UN number	1969
Response guide	115
Hazard class	2.1
USCG CHRIS Code	IBT
USCG Compatatibility Group	31 Paraffins
Std. Transport #	4905747 4905429 4905750
IMO Gas Code	B