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Result for CAS#: 75-28-5

[Expand All \(+\)](#) [Collapse All \(-\)](#)

CAS# found in EINECS (European Inventory of Existing Commercial chemical Substances).

General Information:

EC# : 200-857-2
 CAS# : 75-28-5
 Substance Name : Isobutane
 De : Isobutan
 Es : Isobutano
 Fr : Isobutane
 Molecular Formula : C4H10
 Description : Not available

tBu

[Enlarge Structure](#)

Classification and Labelling Information:

Annex I Index# (1) : 601-004-00-0
 Substance Name : + **Butane**
 in Annex 1 : **And isobutane**
 Note :
 Alphabetic Numeric
 C -
 ATP :
 Inserted Updated
 19 21
 Classification : F+; R12
 Risk Phrases : + **R12 : Extremely flammable.**
 Safety Phrases : + **S2 : Keep out of the reach of children.**
 : + **S9 : Keep container in a well-ventilated place.**
 : + **S16 : Keep away from sources of ignition - No smoking.**

Symbol(s) and Indication(s) of Danger

+ **F+ : Extremely flammable**

Specific Concentration Limit(s) : Not available

Annex I Index# (2) : 601-004-01-8
 Substance Name : + **Isobutane (containing ≥ 0.1 % butadiene (203-450-8))**
 in Annex 1 : **Butane (containing ≥ 0.1 % butadiene (203-450-8))**
 Note :
 Alphabetic Numeric
 CS -

ATP :
 Inserted Updated
 21 28

Classification : F+; R12 - Carc. Cat. 1; R45 - Muta. Cat. 2; R46
 Risk Phrases : + **R45 : May cause cancer.**
 : + **R46 : May cause heritable genetic damage.**
 : + **R12 : Extremely flammable.**
 Safety Phrases : + **S53 : Avoid exposure - obtain special instructions before use.**
 : + **S45 : In case of accident or if you feel unwell, seek medical advice immediately (show the label where possible).**

Symbol(s) and Indication(s) of Danger

+ **F+ : Extremely flammable**+ **T : Toxic**

Specific Concentration Limit(s) : Not available

HPV-LPV (High and Low Production Volume) Information:

HPV Chemical : + **List of Producers/Importers**

IUCLID & OECD Chemical Data Sheets and Export Files Information:

IUCLID Chemical Data Sheet : [view & save it](#)IUCLID Export File : [view & save it](#)

資料IB-9(NIOSH PG)

Isobutane

NIOSH Pocket Guide

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

Chemical Name: Isobutane

Formula: $\text{CH}_3\text{CH}(\text{CH}_3)_2$

Structure/Formula: $\text{CH}_3\text{CH}(\text{CH}_3)_2$

CAS Number: 75-28-5

RTECS Number: TZ4300000

DOT ID and NAERG Guide Numbers: 1075 115
1969 115

2.0 SYNONYMS, TRADENAMES AND CONVERSION FACTORS▲

Synonyms/Tradenames: 2-Methylpropane

Notes: [Also see specific listing for n-Butane.]

Conversion Factor at 68° F and 760 mmHg: 1ppm = 2.38mg/m³

3.0 EXPOSURE LIMITS (TWA UNLESS NOTED OTHERWISE)▲

NIOSH Recommended Exposure Limits (RELs): Time-weighted average (TWA) 800ppm
(1900mg/m³)

OSHA Permissible Exposure Limits (PELs): (Vacated OSHA PELs are listed in Appendix G)
none

4.0 IDLH▲

The IDLH has not been determined.

5.0 PHYSICAL DESCRIPTION▲

Colorless gas with a gasoline-like or natural gas odor.

Notes: [Shipped as a liquefied compressed gas. A liquid below 11° F.]

6.0 CHEMICAL AND PHYSICAL PROPERTIES▲

Molecular Weight: 58.1

Boiling Point: 11° F

Solubility in Water: Slight

Flash Point: NA (Gas)

Ionization Potential: 10.74 eV

Relative Gas Density: 2.06

Flammability Class: Flammable Gas Class IA Flammable Liquid

Vapor Pressure: (70° F) 3.1 atm

Freezing Point: -255° F

Upper Explosive Limit in air (% by volume): 8.4%

Lower Explosive Limit in air (% by volume): 1.6%

7.0 INCOMPATIBILITIES AND REACTIVITIES▲

Strong oxidizers (e.g., nitrates & perchlorates), chlorine, fluorine, (nickel carbonyl + oxygen)

8.0 MEASUREMENT METHOD (SEE TABLE 1)▲

None available

9.0 PERSONAL PROTECTION AND SANITATION (SEE TABLE 3)▲

Skin: Skin: Wear appropriate personal protective clothing to prevent the skin from becoming frozen from contact with the liquid or from contact with vessels containing the liquid.

Eyes: Wear appropriate eye protection to prevent eye contact with the liquid that could result in burns or tissue damage from frostbite.

Wash Skin: No recommendation is made specifying the need for washing the substance from the skin (either immediately or at the end of the work shift).

Remove: Work clothing that becomes wet should be immediately removed due to its flammability hazard (i.e., for liquids with a flash point <100° F).

Change: No recommendation is made specifying the need for the worker to change clothing after the workshift.

Provide: Quick drench facilities and/or eyewash fountains should be provided within the immediate work area for emergency use where there is any possibility of exposure to liquids that are extremely cold or rapidly evaporating.

10.0 RECOMMENDATIONS FOR RESPIRATOR SELECTION (SEE TABLE 4)▲

To be added later.

11.0 HEALTH HAZARDS▲

Exposure Routes: Inhalation, Skin and/or eye contact, (liquid)

Exposure Symptoms (See Table 5): Drowsiness, Narcosis, Asphyxia; liquid: frostbite

Eye (See Table 6): If eye tissue is frozen, seek medical attention immediately; if tissue is not frozen, immediately and thoroughly flush the eyes with large amounts of water for at least 15 minutes, occasionally lifting the lower and upper eyelids. If irritation, pain, swelling, lacrimation, or photophobia persist, get medical attention as soon as possible.

Skin (See Table 6): If frostbite has occurred, seek medical attention immediately; do NOT rub the affected areas or flush them with water. In order to prevent further tissue damage, do NOT attempt to remove frozen clothing from frostbitten areas. If frostbite has NOT occurred, immediately and thoroughly wash contaminated skin with soap and water.

Breath (See Table 6): If a person breathes large amounts of this chemical, move the exposed person to fresh air at once. If breathing has stopped, perform mouth-to-mouth resuscitation. Keep the affected person warm and at rest. Get medical attention as soon as possible.

Target Organs (See Table 5): Central nervous system

ISOBUTANE

資料IB-10(CHRIS)

CHRIS – Chemical Hazard Response Information System

0. OVERVIEW

Material name

ISOBUTANE
CHRIS Code IBT

Common synonyms

2-Methylpropane

Characteristics

Liquefied compressed gas Colorless Odorless
Floats and boils on water. Flammable visible vapor cloud
is produced.

Emergency Actions

Evacuate.
Keep people away.
Shut off ignition sources and call fire department.
Stay upwind and use water spray to ``knock down`` vapor.
Notify local health and pollution control agencies.

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 men effecting shutoff with water.
Let fire burn.

Exposure

CALL FOR MEDICAL AID.
VAPOR
Irritating to eyes.
If inhaled, will cause dizziness, difficult breathing
or loss of consciousness.
Move to fresh air.
If breathing has stopped, give artificial respiration.
If breathing is difficult, give oxygen.
IF IN EYES, hold eyelids open and flush with plenty of water.

Water Pollution – General

Not harmful to aquatic life.

1. CORRECTIVE RESPONSE ACTIONS

Stop discharge
Chemical and Physical Treatment: Burn

2. CHEMICAL DESIGNATIONS

CG Compatibility Group: 31; Paraffin
Formula: $\text{CH}^3\text{CH}(\text{CH}^3)^2$
IMO/UN Designation: 2.0/1969
DOT ID Number: 1969
CAS Registry Number: 75-28-5
NAERG Guide Number: 115
Standard Industrial Trade Classification: 51114

3. HEALTH HAZARDS

Personal Protective Equipment: Self-contained breathing apparatus; safety goggles.
Symptoms Following Exposure: Central nervous system depression ranging from dizziness and incoordination to anesthesia and respiratory arrest, depending on concentration and extent of inhalation. Irregular heartbeat is rare but is a dangerous complication at anesthetic levels.
Treatment of Exposure: INHALATION: protect victim against self-injury if he is stuporous, confused, or anesthetized; apply artificial respiration if breathing has stopped; avoid administration of epinephrine or other sympathomimetic amines; prevent aspiration of vomitus by proper positioning of head; give symptomatic and supportive treatment. INGESTION OR ASPIRATION: no treatment required.
TLV-TWA: Not listed.
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 skin because it is very volatile and evaporates quickly. Some frostbite possible.
Odor Threshold: Currently not available
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: -117° 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: 890° F
Electrical Hazard: Not pertinent
Burning Rate: 9.3 mm/min.

Adiabatic Flame Temperature: Currently not available
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: Pure; technical
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: 10.8° F = -11.8° C = 261.4° K
Freezing Point: -427.5° F = -255.3° C = 17.9° K
Critical Temperature: 275° F = 135° C = 408° K
Critical Pressure: 529 psia = 36.0 atm = 3.65 MN/m²

Specific Gravity: 0.557 at 20° C (liquid)
Liquid Surface Tension (Est.): 14 dynes/cm = 0.014 N/m at -10° C
Liquid Water Interfacial Tension: (est.) 50 dynes/cm = 0.05 N/m at -10° C
Vapor (Gas) Specific Gravity: 2.0
Ratio of Specific Heats of Vapor (Gas): 1.095
Latent Heat of Vaporization: 158 Btu/lb = 87.5 cal/g = 3.66×10^5 J/kg
Heat of Combustion: -19,458 Btu/lb = -10,810 cal/g = -452.59×10^5 J/kg
Heat of Decomposition: Not pertinent
Heat of Solution: Not pertinent
Heat of Polymerization: Not pertinent
Heat of Fusion: 18.96 cal/g
Limiting Value: Currently not available
REID Vapor Pressure: Currently not available

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	
						(7a)	(7b)	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 CHLOROPENTAFLUOROETHANE 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

ALIPHATIC HYDROCARBONS

5.0 2-Methylpropane

5.0.1 CAS Number: [75-28-5]

5.0.2 Synonyms: Isobutane, various grades; 1,1-dimethylethane; trimethylmethane

5.0.3 Trade Names: NA

5.0.4 Molecular Weight: 58.12

5.0.5 Molecular Formula: $\text{CH}(\text{CH}_3)_3$

5.0.6 Molecular Structure:



5.1 Chemical and Physical Properties

5.1.1 General

2-Methylpropane (isobutane), C_4H_{10} , a flammable gas, occurs in small quantities in natural gas and crude oil. It has been detected in urban atmospheres at concentrations of 44–74 ppb (68, 69). It also evolves from natural sources and has been measured in diesel exhaust (70, 71) and in cigarette smoke (72). Selected physical properties are listed in Table 49.1.

5.1.2 Odor and Warning Properties

Isobutane has a gasoline-like or natural gas odor (36).

5.2 Production and Use

Isobutane is produced in petroleum refining processes and from raw natural gas (73). It is used as a component of gasoline and in the blending of motor fuels, in the production of high octane blend stocks, as a refrigerant and aerosol propellant in cosmetic and other consumer products, as a constituent of liquefied natural gas and substitute natural gas, and in the synthesis of other chemicals (e.g., propylene oxide and propylene glycol) and products such as polyurethane foams and resins (73).

5.3 Exposure Assessment

5.3.1 Air

Headspace gas chromatography and infrared absorption spectroscopy have been used to measure isobutane concentrations in exposure chamber atmospheres (74). A gas chromatographic method for identification of propellants and aerating agents in aerosol whipped toppings and antistick pan coatings has been developed (75).

5.3.2 Background Levels: NA

5.3.3 Workplace Methods: NA

5.3.4 Community Methods: NA

5.3.5 Biomonitoring/Biomarkers

Isobutane has been determined in blood and expired air of human volunteers by headspace gas chromatography (74).

5.4 Toxic Effects

5.4.1 Experimental Studies

5.4.1.1 Acute Toxicity. The I-h LC₅₀ for the mouse is 52 mg/L (42). At concentrations in the range of the LC₅₀, mice exhibit CNS depression, rapid and shallow respiration, and apnea (5). In another study, 2-h exposures of mice to 41 mg/L caused death in 60% of the exposed animals, whereas exposure to 52 mg/L was lethal to 100% of the animals within an average of 28 min (60). In dogs, 55 mg/L were fatal, and 45 mg/L caused anesthesia (60).

5.4.1.2 Chronic and Subchronic Toxicity. Subchronic toxicity studies of exposure to mixtures containing isobutane are summarized in Table 49.6 (46, 76, 77).

5.4.1.3 Pharmacokinetics, Metabolism, and Mechanisms. Isobutane is oxidatively metabolized by rat liver microsomes to its parent alcohol (30). Butanol cannot be oxidized to a ketone product, and it may be either conjugated with glucuronic acid or excreted unchanged in the expired air or urine (78).

5.4.1.4 Reproductive and Developmental: NA

5.4.1.5 Carcinogenesis: NA

5.4.1.6 Genetic and Related Cellular Effects Studies. Isobutane tested negative in the Ames *Salmonella* mutagenicity assay (64).

5.4.1.7 Other: Neurological, Pulmonary, Skin Sensitization, etc. Isobutane is a weak cardiac sensitizer (42, 65). At high concentrations, a decrease in pulmonary compliance and tidal volume has been noted in the rat (79). No effects were noted in anesthetized dogs at concentrations of $\leq 2\%$, but decreased myocardial contractility was noted at 2.5%; exaggerated effects, at 5%, with a decrease in ventricular and aortic pressure; and at 10%, decreased left ventricular pressure, mean arterial flow, and stroke volume, with increased pulmonary vascular resistance. Isobutane is a CNS depressant in the mouse at 15% in 60 min, and at 23% in 26 min (60). Studies in rabbits exposed in the eyes to undiluted hairspray containing 22% isobutane, showed that irritation of the eye was immediately evident with transient iritis and mild conjunctivitis (73).

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Table 49.6. Summary of Subchronic Toxicity Studies in Animals Exposed to Mixtures Containing 2-Methylpropane

Species	Exposure route	Chemical mixture	Approximate Dose	Treatment regimen	Observed Effect	Ref.
Fischer rats	Inhalation	50-50 (wt%) <i>n</i> -butane: <i>n</i> -pentane	1000, 4500 ppm	6 h/day, 5 days/ week, 13 weeks	Mild-transient kidney effects not exposure-related	76
		50-50 (wt %) isobutane: isopentane	1000, 4500 ppm	6 h/day, 5 days/ week, 13 weeks	Mild-transient kidney effects not exposure-related	
		Unleaded gasoline blend	1200, 5200 ppm	6 h/day, 5 days/ week, 13 weeks	No nephrotoxicity observed	
Sprague-Dawley rats	Inhalation	25 (wt%) <i>n</i> -butane, <i>n</i> - pentane, isobutane, iso- pentane	0, 44, 432, 4437 ppm	6 h/day, 5 days/ week, 3 weeks	No clinical signs of toxicity and no nephrotoxicity observed	77
		Rabbits	Inhalation	Hairspray with 22% iso- butane	2 daily — 30-s aero- sol bursts	3 days/week, 90 days

5.4.2 Human Experience

5.4.2.1 General Information. Isobutane is a simple asphyxiant. Acute exposures may cause tachypnea and tachycardia. In severe cases, hypotension, apnea, and cardiac arrest develop. Direct contact with the liquid produces chemical burns. Toxicologically, the vapor exerts no effect on skin and eyes (5).

5.4.2.3 Epidemiology Studies

5.4.2.3.1 Acute Toxicity. Human volunteers exposed to 250–1000 ppm for 1 min to 8 h and 500 ppm for 1–8 h/day for 10 days to isobutane showed no adverse effects or abnormal physiological responses (cardiac and pulmonary function) (53, 74).

5.5 Standards, Regulations, or Guidelines of Exposure

Isobutane is on the EPA TSCA Chemical Inventory and the Test Submission Data Base (16). The NIOSH 10-h TWA is 800 ppm (1900 mg/m³) (36). Table 49.7 shows the occupational exposure limits for isobutane in different countries.

6.0 n-Pentane

6.0.1 CAS Number: [109-66-0]

6.0.2 Synonyms: Amyl hydride, skellysolve A, normal pentane

6.0.3 Trade Names: NA

6.0.4 Molecular Weight: 72.15

6.0.5 Molecular Formula: CH₃(CH₂)₃CH₃

6.0.6 Molecular Structure: 

Table 49.7. Occupational Exposure Limits for 2-Methylpropane in Different Countries^a

Country	Exposure Limit
Germany	TWA 1000 ppm (2350 mg/m ³)
Switzerland	TWA 800 ppm (1900 mg/m ³)
United Kingdom	TWA 600 ppm (1430 mg/m ³); STEL 750 ppm

^aFrom Ref. 19.

(Patty's, vol. w)

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 <i>n</i> _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 ₂ H ₆	30.07	-88.63	-183.23	0.5446 (-89)	—	bz 4	-135	3.0-12.5
Propane	C ₃ H 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 ₄ H 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 ₄ H 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 ₅ H 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 ₅ H 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 ₆ H 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 ₆ H 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 ₅ H 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 ₆ H 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 ₆ H 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 ₆ H 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 ₇ H 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 ₇ H 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 ₇ H 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 ₈ H 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)	1.0-6.5

22

(open cup)

2516 MOR250 METHYL POTASSIUM

mf: $C_{20}H_{29}NO_3$ mw: 331.50SYNS: N-METHYL-3-PIPERIDYL- α -CYCLOHEXYL
MANDELATE \square OXYCLIPINE

TOXICITY DATA with REFERENCE:

ivn-rat LD50:18 mg/kg AIPTAK 120,186,59

ivn-mus LD50:32 mg/kg AIPTAK 120,186,59

SAFETY PROFILE: Poison by intravenous route.
When heated to decomposition it emits toxic fumes of NO_x .MOR250 CAS: 17814-73-2 HR: 3
METHYL POTASSIUMmf: CH_3K mw: 54.13SAFETY PROFILE: Since it is incompatible with
moisture (as in all living tissue), it must be considered a
poison. When dry it ignites spontaneously in air. When
heated to decomposition it emits toxic fumes of K_2O . See
also POTASSIUM COMPOUNDS.MOR500 CAS: 83-43-2 HR: 2
METHYLPREDNISOLONEmf: $C_{22}H_{30}O_5$ mw: 374.52

PROP: Crystals. Mp: 228-237°.

SYNS: MEDROL \square MEDROL DOSEPAK \square MEDRONE \square Δ^1 -6-
 α -METHYLHYDROCORTISONE \square 6- α -METHYLPREDNISOL-
ONE \square METRISONE \square NSC-19987 \square 11- β ,17,21-TRIHYDROXY-6-
 α -METHYLPREGNA-1,4-DIENE-3,20-DIONE \square 11- β ,17- α ,21-
TRIHYDROXY-6- α -METHYL-1,4-PREGNADIENE-3,20-DIONE \square
URBASON \square URBASONE \square WYACORT

TOXICITY DATA with REFERENCE:

par-wmn TDLo:2400 μ g/kg:CVS BJANAD 69,422,92ivn-wmn TDLo:60 mg/kg/3D-I:CVS,SYS AIMBAS
99,282,83ivn-wmn TDLo:20 mg/kg/45M-C:CVS,PUL JRHUA9
13,477,86

ipr-mus LD50:2292 mg/kg NIIRDN 6,832,82

CONSENSUS REPORTS: Reported in EPA TSCA
Inventory.SAFETY PROFILE: Moderately toxic by
intrapertoneal route. A steroid hormone. Human
systemic effects include arrhythmias, blood pressure
lowering, heart rate changes, increased body temperature,
pulse rate increase, respiratory depression. When heated to
decomposition it emits acrid smoke and irritating fumes.MOR600 CAS: 90350-40-6 HR: D
METHYLPREDNISOLONE SULEPTANATEmf: $C_{33}H_{49}NO_{10}S \cdot Na$ mw: 673.87SYNS: PREGAN-1,4-DIENE-3,20-DIONE, 11,71-DIHYDROXY-6-
METHYL-21-((8-(METHYL(2-SULFOETHYL) AMINO)-1,8-
DIOXOOCCTYL)OXY)-, MONOSODIUM SALT, (6- α -11- β)- \square U-
67,590ASAFETY PROFILE: Experimental reproductive
effects. When heated to decomposition it emits toxic
vapors of NO_x .MOR750 CAS: 75-28-5 HR: 3
2-METHYLPROPANE

DOT: UN 1969

mf: C_4H_{10} mw: 58.14PROP: Colorless gas. Fp: -145°, bp: -10.2°, lcl: 1.9%,
uel: 8.5%, d: 0.5572 @ 20°, autoign temp: 864°F, vap d:
2.01. Sol in EtOH, Et₂O, and $CHCl_3$; spar sol in H_2O .SYNS: ISOBUTANE \square ISOBUTANE (DOT) \square ISOBUTANE
MIXTURES (DOT)

TOXICITY DATA with REFERENCE:

ihl-rat LC50:57 pph/15M HUTODJ 1,239,82

ihl-mus LCLo:1041 $g/m^3/2H$ JPETAB 58,74,36CONSENSUS REPORTS: Reported in EPA TSCA
Inventory.DFG MAK: 1000 ppm (2400 mg/m^3)

DOT CLASSIFICATION: 2.1; Label: Flammable Gas

SAFETY PROFILE: An asphyxiant. A common air
contaminant. A very dangerous fire and explosion hazard
when exposed to heat, flame, or oxidizers. To fight fire,
stop flow of gas. When heated to decomposition it emits
acrid smoke and irritating fumes.MOS000 CAS: 75-66-1 HR: 3
2-METHYL-2-PROPANETHIOLmf: $C_4H_{10}S$ mw: 90.20PROP: Mobile liquid; heavy skunk odor. Mp: -0.5°, bp:
63.7-64.2°, d: 0.79-0.82 @ 15.5°/15.5°, flash p: <-20°F
vap d: 3.1, n: (25/D) 1.41984. Sldly sol in water; very sol in
alc, ether, and liquid H_2S .SYNS: tert-BUTANETHIOL \square tert-BUTYL MERCAPTAN

TOXICITY DATA with REFERENCE:

eye-rbt 84 mg AIHAAP 19,171,58

oxl-rat LD50:4729 mg/kg AIHAAP 19,171,58

ihl-rat LC50:22,200 ppm/4H AIHAAP 19,171,58

ipr-rat LD50:590 mg/kg AIHAAP 19,171,58

CONSENSUS REPORTS: Reported in EPA TSCA
Inventory.SAFETY PROFILE: Moderately toxic by
intrapertoneal route. Mildly toxic by ingestion. An eye
irritant. A very dangerous fire hazard when exposed to
heat or flame. Can react vigorously with oxidizing
materials. To fight fire, use alcohol foam, dry chemical
mist, fog. When heated to decomposition or on contact
with acid or acid fumes it emits highly toxic fumes of S_2 .
See also MERCAPTANS.MOS100 CAS: 1843-03-4 HR: 1
4,4',4''-(1-METHYL-1-PROPANYL-3-YLIDENE)
TRIS(2-(1,1-DIMETHYLETHYL)-5-METHYL-
PHENOL)mf: $C_{37}H_{52}O_3$ mw: 544.89SYNS: m-CRESOL, 4,4',4''-(1-METHYL-1-PROPANYL-3-YLID-
ENE)TRIS(6-tert-BUTYL)-(7Cl,8Cl) \square GSY 930 \square MARK AO
PHENOL, 4,4',4''-(1-METHYL-1-PROPANYL-3-YLIDENE)TRIS
(1,1-DIMETHYLETHYL)-5-METHYL)- \square TOPANOL CA \square TRIS
 \square TRISALKOFEN BMB

TOXICITY DATA with REFERENCE:

unr-uns LD50:16,100 mg/kg GISAAA 42(7),74,77

CONSENSUS REPORTS: Reported in EPA TSCA
Inventory.SAFETY PROFILE: Low toxicity by an unspecified
route. When heated to decomposition it emits acrid
and irritating vapors.

MOS250 CAS: 555-57-7 HR: 3

Chemical Name Formula (Synonym) CAS No.	NFPA 30/ OSHA Class	Flash Point °F(°C)	Ignition Temp. °F(°C)	Flammable Limits		Sp.Gr. (Water = 1)	Vapor Density (Air = 1)	Boiling Point °F(°C)	Water Soluble	Extinguishing Methods	Hazard Identification		
				Percent by Vol.							Health	Flamma- bility	Insta- bility
				Lower	Upper								
α -Ioneone $C(CH_3)_2CH_2CH_2$ CH ₂ C(CH ₃)CHCH ₂ CHC(CH ₃)=O (α -Cycloclry- lideneacetone) [4-(2,6,6-Trimethyl-2- Cyclohexan-1-yl)-3- Buten-2-one]	IIIB	>212 (>100)				0.9		259-262 (126-128) @ 12 mm	Slight	5 2	1	0	
β -Ioneone $C(CH_3)_2CH_2CH_2CH_2C-$ (CH ₃)=CCHCHC- (CH ₃)=O (β -Cycloclry- lideneacetone) [4-(2,6,6-Trimethyl-1- Cyclohexan-1-yl)-3- Buten-2-one] 14901-07-6	IIIB	>212 (>100)				0.9		284 (140) @ 18 mm	No	5 2	1	0	
Iron Carbonyl Fe(CO) ₅ 13463-40-6	IB	5 (-15)				1.45	6.74	221 (105)			1	3	1
Isano Oil							1.0-					1	3
Note: Exothermic reaction above 502 (261); may become explosive.													
Isamyl Acetate $CH_3COOCH_2CH_2CH-$ (CH ₃) ₂ (Banana Oil) (3-Methyl-1-Butanol Acetate) (2-Methyl Butyl Etha- noate) 123-82-2	IC	77 (25)	680 (350)	1.0 @ 212 (100)	7.5	0.9	4.5	290 (143)	Slight	5 1	1	3	0
Isamyl Alcohol (CH ₃) ₂ CHCH ₂ CH ₂ OH (Isobutyl Carbinol) (Fusel Oil) (3-Methyl-1-Butanol) 123-51-3	II	109 (43)	662 (350)	1.2	9.0 @ 212 (100)	0.8	3.0	270 (132)	Slight	5	1	2	0
tert-Isamyl Alcohol	See 2-Methyl-2-Butanol.												
Isamyl Butyrate $C_2H_5CO_2(CH_2)_2CH(CH_3)_2$ (Isopentyl Butyrate) 106-27-4	II	138 (59)				0.88	5.45	352 (178)			1	2	0
Isamyl Chloride (CH ₃) ₂ CHCH ₂ CH ₂ Cl (1-Chloro-3- Methylbutane) 107-84-6	IB	<70 (<21)		1.5	7.4	0.89	3.67	212 (100)		1		3	
Isamyl Nitrite $CH_3(CH_2)_2NO_2$ (Amyl nitrite) 110-46-3	IB	50 (10)	410 (210)			0.9	4.0	220 (104)	Slight	5	2	3	2
Isobornyl Acetate $C_{10}H_{17}OOCCH_3$ 125-12-2	IIIA	190 (88)				1.0-		428-435 (220-224)	No	5	1	2	0
Isobutane (CH ₃) ₂ CH (2-Methylpropane) 75-28-5		Gas	860 (450)	1.8	8.4		2.0	11 (-12)	No	6	0	4	0
Isobutyl Acetate $CH_3COOCH_2CH(CH_3)_2$ (β -Methyl Propyl Etha- noate) 110-19-0	IB	64 (18)	790 (421)	1.3	10.5	0.9	4.0	244 (118)	No	5 1	1	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
6354	α-lone	4-(2,5,6-Tetramethyl-2-cyclohexen-1-yl)-3-buten-2-one	C ₁₁ H ₂₀ O	79-69-6	206.324			90 ^g	0.9352 ²⁰	1.5002 ²⁰	
6355	β-lone	4-(2,5,6-Tetramethyl-1-cyclohexen-1-yl)-3-buten-2-one	C ₁₁ H ₂₀ O	79-70-9	206.324		125 ¹¹		0.9434 ¹¹	1.5162 ¹¹	s H ₂ O; vs EOH, eth, bz, chl
6356	Iron hydroxycarbonyl	Hydrogen tetracarboxylate(II)	C ₄ H ₂ FeO ₇	17440-80-3	169.902	col liq, unstab	-70				s alk
6357	Iron nonacarbonyl	Diron nonacarbonyl	C ₉ F ₈ O ₄	15321-51-4	363.781	oran-ye cry	100 dec		2.85		s H ₂ O
6358	Iron(III) NTA	Nitrotriacetateiron(III)	C ₆ H ₄ FeNO ₆	18448-54-7	243.960	solid					
6359	Iron pentacarbonyl	Iron pentacarbonyl	C ₅ FeO ₅	13463-40-6	195.866	col to ye oily liq	-20	103	1.5 ¹⁰	1.4632 ¹⁰	s H ₂ O; sl EOH; s bz, ace, chl
6360	Iron(III) 2,4-pentanedioate	Ferric acetylacetonate	C ₁₂ H ₁₂ FeO ₆	14824-18-1	363.169		179		5.24		
6361	Isaric acid	17-Octadecene-9,11-dienoic acid	C ₁₈ H ₃₂ O ₂	506-25-2	274.398	cr	39.5		0.9308 ⁹	1.4914 ⁹	s ace, EOH, l-FrOH; sl peth
6362	Isaldine	Retrosine A-oxide	C ₁₇ H ₂₈ NO ₂	15503-86-3	307.395	cr	146				
6363	Isaxamine	N-Isopropyl-2-pyrimidinamine	C ₈ H ₁₀ N ₂	4214-72-6	137.182		28	93 ¹⁸			
6364	Isazophos	C ₃ H ₇ CN ₂ O ₂ S	67329-04-8	313.741				170; 100 ^{mm}	1.22 ²⁰		
6365	Isobenzan	C ₈ H ₁₀ Cl ₂ O	287-78-9	417.751		cr (mp)	121				s eth, bz, xyl, tol
6366	1(3 <i>H</i>)-Isobenzothiazinone	C ₆ H ₄ O ₂	87-41-2	134.133		nl or pl (w)	75	230	1.163 ⁹	1.539 ⁹	s H ₂ O; vs EOH, eth; sl chl
6367	Isoborneol	1,7,7-Trimethylbicyclo[2.2.1]heptan-2-ol, exo-(<i>±</i>)	C ₁₀ H ₁₈ O	24833-70-2	154.249	tab (peth)	212	sub	1.10 ⁹		s H ₂ O; vs EOH, eth, chl; sl bz
6368	Isobornyl thiocyanate	C ₁₁ H ₁₈ N ₂ S	115-31-1	253.351		ye oily liq		95 ^{mm}	1.1465 ⁵	1.512 ⁵	s H ₂ O; vs EOH, bz, chl, peth
6369	5-Isobornyl-3,4-xylene	Xibornol	C ₁₇ H ₂₆ O	13741-18-9	258.399	cr	85	167 ¹	1.0240 ²⁰	1.5382 ²⁰	
6370	Isobutanal	2-Methyl-1-propanal	C ₄ H ₈ O	78-84-2	72.106	liq	-85.9	64.5	0.7891 ¹⁰	1.3730 ¹⁰	s H ₂ O, eth, ace, chl; sl chl
6371	Isobutane	2-Methylpropane	C ₄ H ₁₀	75-28-5	58.122	col gas	-159.4	-11.73	0.5510 ²⁵ (p>1 atm)	1.3618 ²⁵	sl H ₂ O; s EOH, eth, chl
6372	Isobutene	C ₄ H ₈	115-11-7	56.107		col gas	-140.7	-6.9	0.599 ²⁵ (p>1 atm)	1.3928 ²⁵	s H ₂ O; vs EOH, eth; s bz, sul
6373	Isobutyl acetate	C ₆ H ₁₂ O ₂	110-19-0	116.158		liq	-99.8	116.5	0.8712 ²⁰	1.392 ²⁰	sl H ₂ O, chl; msc EOH, eth; s ace
6374	Isobutyl acrylate	C ₆ H ₁₀ O ₂	106-63-8	128.169		liq	-61	132	0.8896 ²⁰	1.4150 ²⁰	sl H ₂ O; s EOH, eth, MeOH
6375	5-Isobutyl-3-allyl-2-thioxo-4-imidazolimidone	Albutoin	C ₁₇ H ₂₆ N ₂ O ₂ S	830-89-7	272.311		210.5				
6376	Isobutyramine	2-Methyl-1-propanamine	C ₄ H ₁₁ N	78-81-9	73.137	liq	-85.7	67.75	0.724 ⁸	1.3980 ¹⁹	
6377	Isobutyl 4-aminobenzoate	Isobutyl p-aminobenzoate	C ₁₁ H ₁₃ N ₂ O ₂	94-14-4	193.243		64.5				
6378	Isobutylbenzene	C ₉ H ₁₄	538-88-2	134.218		liq	-51.4	172.79	0.8532 ²⁰	1.4685 ²⁰	s H ₂ O; msc EOH, eth, ace, bz, peth, chl
6379	Isobutyl benzoate	C ₁₁ H ₁₄ O ₂	120-50-3	178.228			242		0.960 ²⁰		s H ₂ O; msc EOH, eth; s ace, chl
6380	Isobutyl butanoate	C ₈ H ₁₆ O ₂	539-90-2	144.212			155.9		0.8364 ¹⁸	1.4032 ²⁰	sl H ₂ O; msc EOH, eth
6381	Isobutyl carbamate	C ₆ H ₁₁ N ₂ O ₂	543-28-2	117.147		lf	67			1.4038 ²⁰	vs eth, EOH
6382	Isobutyl chlorocarbonate	C ₆ H ₁₁ ClO ₂	543-27-1	136.577			128.8		1.1426 ¹⁴	1.4071 ¹⁴	s EOH, bz, chl; msc eth
6383	Isobutyl 2-chloropropanoate	C ₇ H ₁₃ ClO ₂	114489-96-2	164.630			176		1.0312 ²⁰	1.4247 ²⁰	
6384	Isobutyl 3-chloropropanoate	C ₇ H ₁₃ ClO ₂	62108-88-3	164.630			191.3		1.0323 ²⁰	1.4295 ²⁰	vs eth, EOH
6385	Isobutylcyclohexane	C ₁₀ H ₁₈	1678-99-4	140.266		liq	-95	171.3	0.7952 ²⁰	1.4362 ²⁰	s H ₂ O; s EOH, ace, chl; vs eth, bz
6386	Isobutylcyclopentane	C ₉ H ₁₆	3788-32-7	128.239		liq	-115.2	148	0.7768 ²⁰	1.4298 ²⁰	
6387	Isobutyl dimethylamine	N,N,2-Trimethyl-1-propanamine	C ₆ H ₁₃ N	7238-24-9	101.190		60.5		0.7097 ¹⁸	1.3507 ²⁰	vs H ₂ O
6388	Isobutyl formate	C ₅ H ₁₀ O ₂	542-85-2	102.132		liq	-95.8	98.2	0.8776 ²⁰	1.3857 ²⁰	sl H ₂ O, chl; msc EOH, eth; vs ace
6389	Isobutyl heptanoate	Isobutyl enanthate	C ₁₁ H ₂₀ O ₂	7779-80-8	186.282		208		0.8553 ¹⁹		vs ace, bz, eth, EOH
6390	Isobutyl 2-hydroxybenzoate	Isobutyl salicylate	C ₁₁ H ₁₄ O ₃	87-19-4	184.227		281		1.0639 ²⁰	1.5087 ²⁰	s H ₂ O; s EOH, eth, chl
6391	Isobutyl isobutanoate	C ₈ H ₁₆ O ₂	97-85-8	144.212		liq	-80.7	148.6	0.8542 ²⁰	1.3939 ²⁰	sl H ₂ O, chl; s EOH, ace; msc eth
6392	Isobutyl isopropylate	C ₉ H ₁₈ O	1879-29-6	99.131			106			1.5005 ¹⁴	
6393	Isobutyl isobutyrate	1-Isobutyryloxypropane	C ₈ H ₁₆ O ₂	581-82-2	115.197		160				