

ACE4750

CAS #: 67-64-1

ACETONE

RTECS: AL3150000

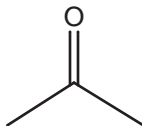
DOT: UN1090; IMO3.1

EINECS Number: 200-662-2

Molecular Formula: C₃H₆O

Structured MF: CH₃COCH₃

Formula Weight: 58.09



Chemical Structure

Synonyms: ACETON; CHEVRON ACETONE; DIMETHYL KETONE; DIMETHYLFORMALDEHYDE; DIMETHYLKETAL; EPA PESTICIDE CHEMICAL CODE 004101; KETONE PROPANE; KETONE,DIMETHYL; BETA-KETOPROPANE; METHYL KETONE; 2-PROPANONE; PROPANONE; PYROACETIC ACID; PYROACETIC ETHER

Description: colorless liquid; sweetish odor

Use: in the manufacture of smokeless powder, paints, varnishes, lacquers, organic chemicals, pharmaceuticals, sealants, adhesives, methyl isobutyl ketone, mesityl oxide, acetic acid (ketene process), diacetone alcohol, chloroform, iodoform, bromoform, explosives, airplane dopes, rayon, photographic films, isoprene, methyl isobutyl carbinol, methyl methacrylate and bisphenol A; as solvent for cellulose acetate, nitrocellulose, acetylene, fats, oils, waxes, resins, rubber, plastics, rubber cements, pharmaceuticals, potassium iodide and permanganate; in storing acetylene gas, in purifying paraffin, in hardening and dehydrating tissues and to clean and dry parts of precision equipment; in extraction of various principles from animal and plant substances, as a delusterant for cellulose acetate fibers, in specification testing of vulcanized rubber products, as a cosmetic ingredient, as a dye intermediate and in paint and varnish removers

Physical Properties

Boiling Point: 56.2 °C (133 °F) at 760 mm Hg

Freezing Point: -95.35 °C (-139.63 °F)

Specific Gravity: 0.7899 at 20 °C/4 °C

Vapor Density: 2 Air=1

Saturated Vapor Density: 1.565868784 kg/m³

Density: 0.786 gm/cc at 22.7 °C

Vapor Pressure: 231 mm Hg at 25 °C

Water Solubility: Miscible

Other Solubilities: 95% Ethanol: >=100 mg/ml at 22 °C; Acetone: >=100 mg/ml at 22 °C;

Benzene: Soluble; Chloroform: miscible; DMSO: >=100 mg/ml at 22 °C; Ether: miscible;

Methanol: miscible; Most oils: miscible; Organic solvents: miscible.

Surface Tension: 26.2 nM/M at 0 °C

Odor Threshold: 47.5 to 1613.9 mg/m³

Refraction Index: 1.3588 at 20 °C/D

Evaporation Rate: < 1 Butyl Acetate=1

Critical Temperature: 235 °C

Critical Pressure: 46.4 atm

Ionization Potential (eV): 9.69

Flash Point: -20 °C

Autoignition Temperature: 465 °C

LEL: 2.15% v/v

UEL: 13% v/v

RTECS Toxicity Data

Acute Oral: Man TD_{Lo} Dose: 2857 mg/kg; Toxic Effects: Behavioral - Coma; Kidney, Ureter, and Bladder - Other changes. Man TD_{Lo} Dose: 2857 mg/kg; Toxic Effects: Behavioral - Coma; Biochemical - Other. Rat LD₅₀ Dose: 5800 mg/kg; Toxic Effects: Behavioral - Altered sleep time (including change in righting reflex); Behavioral - Tremor.

Acute Inhalation: Rat LC₅₀ Dose: 50100 mg/m³/8hr. Human TC_{Lo} Dose: 500 ppm; Toxic Effects: Sense organs and special senses - Other; Sense organs and special senses - Conjunctive irritation; Lungs, Thorax, or Respiration - Other changes. Man TC_{Lo} Dose: 440 ug/m³/6M; Toxic Effects: Brain and coverings - Recordings from specific areas of CNS. Man TC_{Lo} Dose: 10 mg/m³/6hr; Toxic Effects: Biochemical - Other carbohydrates. Man TC_{Lo} Dose: 12000 ppm/4hr; Toxic Effects: Gastrointestinal - Nausea or vomiting; Behavioral - Muscle weakness.

Acute Dermal: Rabbit LD_{Lo} Route: Skin; Dose: 20 mL/kg. Guinea Pig LD₅₀ Route: Skin; Dose: >9400 mg/kg.

Chronic (Multiple Dose) Oral: Rat Dose: 273 gm/kg/13W-C; Toxic Effects: Liver - Changes in liver weight; Kidney, Ureter, and Bladder - Changes in kidney weight; Blood - Normocytic anemia. Mouse Dose: 546 gm/kg/13W-C; Toxic Effects: Liver - Changes in liver weight; Endocrine - Changes in spleen weight.

Chronic (Multiple Dose) Inhalation: Rat Dose: 19000 ppm/3H/8W-I; Toxic Effects: Brain and coverings - Changes in brain weight. Rat Dose: 199 mg/m³/8H/45D-I; Toxic Effects: Behavioral - Muscle contraction or spasticity.

Irritation Eye: Rabbit Standard Draize Test Dose: 20 mg/24H; Reaction: moderate. Rabbit Standard Draize Test Dose: 20 mg; Reaction: severe.

Irritation Skin: Rabbit Standard Draize Test Dose: 500 mg/24H; Reaction: mild. Rabbit Open Draize Test Dose: 395 mg open; Reaction: mild.

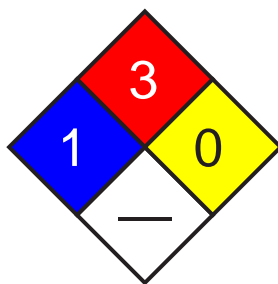
Reproductive/Teratogenic: Rat Route: Oral; Dose: 273 gm/kg; Duration: male 13W prior to mating; Paternal Effects - Spermatogenesis. Mammal Route: Inhalation; Dose: 31500 ug/m³/ Duration: female 1-13D of pregnancy; Effects on Fertility - Post-implantation mortality.

Mutagenic: Hamster Cytogenetic Analysis; Cell Type: fibroblast; Dose: 40 gm/L. Yeast - S Cerevisiae Sex Chromosome Loss; Dose: 47600 ppm.

Hazard Overviews



Flammable



Fire Diamond

Health: Irritating to eyes/skin/respiratory tract. Also Causes: muscle weakness, mental confusion, coma (high concentrations) ingestion: GI irritation, kidney and liver damage, metabolic changes, coma. Chronic Effects: dermatitis.

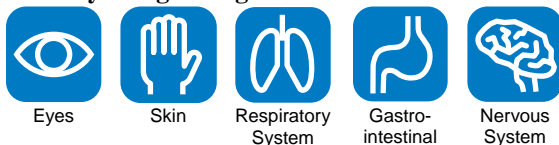
Fire: Flammable. Can form explosive mixtures in the air. Do not extinguish fire unless flow can be stopped. For small fires, use dry chemical, carbon dioxide, water spray or alcohol-resistant foam. For large fires, use water spray, fog, or alcohol-resistant foam. Use water in flooding quantities as fog because solid streams may be ineffective.

Reactivity: Stable. Hazardous polymerization cannot occur. Avoid: contact with plastic eyeglass frames, jewelry, pens, pencils, and rayon garments. Incompatible with: hydrogen peroxide; acetic acid; nitric acid; nitric acid and sulfuric acid; chromic anhydride; chromyl chloride; nitrosyl chloride; hexachloromelamine; nitrosyl perchlorate; nitryl perchlorate; permonosulfuric acid;

thiodiglycol and hydrogen peroxide; oxidizing materials; activated carbon; chromium trioxide; dioxygen difluoride and carbon dioxide; potassium-tert-butoxide; air; bromoform; bromine; chloroform and alkalis; trichloromelamine; sulfur dichloride. Hazardous decomposition products: carbon dioxide; carbon monoxide.

Carcinogenicity: IARC - Not listed; NIOSH - Not listed; NTP - Not listed; ACGIH - Not listed; OSHA - Not listed; EPA - Class D, Not classifiable as to human carcinogenicity; MAK - Not listed

Primary Target Organs:



Exposure Limits

OSHA PEL: TWA: 1000 ppm; 2400 mg/m³.

OSHA PEL Vacated 1989 Limits: TWA: 750 ppm; 1800 mg/m³; STEL: 1000 ppm; 2400 mg/m³.

ACGIH TLV: TWA: 750 ppm; 1780 mg/m³; STEL: 1000 ppm; 2380 mg/m³.

NIOSH REL: TWA: 250 ppm; 590 mg/m³.

NIOSH IDLH: 2500 ppm; LEL.

DFG MAK: TWA: 500 ppm; 1200 mg/m³.

Respirator Recommendation

Exposure Range: >1000 to <2500 ppm Supplied Air, Constant Flow/Pressure Demand, Full Face

Exposure Range: 2500 to unlimited ppm Self-contained Breathing Apparatus, Pressure Demand, Full Face

Note: use ov (black) cartridge for nuisance(<1000)

Environmental

Ecotoxicity: LD₁₀₀ *Asellus aquaticus* 3 ml/l (within 3 days of exposure) /Conditions of bioassay not specified LC₅₀ Mexican axolotl 20.0 mg/l/48 hr (3-4 weeks after hatching) /Conditions of bioassay not specified TLm Mosquito fish 13,000 mg/l/24, 48, 96 hr /Conditions of bioassay not specified LD₁₀₀ *Gammarus fossarum* 10 ml/l (within 48 hr) /Conditions of bioassay not specified LC₅₀ *Poecilia reticulata* (guppy) 7,032 ppm/14 days /Conditions of bioassay not specified LC₅₀ Ring-necked pheasant oral greater than 40,000 ppm, in diet, age 10 days, (no mortality to 40,000 ppm) LC₅₀ *Salmo gairdneri* (Rainbow trout) 5,540 mg/l/96 hr at 12 °C (95% confidence limit 4,740-6,330 mg/l), wt 1.0 g /static bioassay LC₅₀ Clawed toad 24.0 mg/l/48 hr (3-4 weeks after hatching) /Conditions of bioassay not specified TLm *Daphnia magna* 10 mg/l/24, 48 hr /Conditions of bioassay not specified

Environmental Fate: If released on soil, it will both volatilize and leach into the ground and probably biodegrade. If released into water, it will probably biodegrade. It will also be lost due to volatilization (estimated half-life 20 hr from a model river). Bioconcentration in aquatic organisms and adsorption to sediment should not be significant. In the atmosphere, it will be lost by photolysis and reaction with photochemically produced hydroxyl radicals. Half-life estimates from these combined processes average 22 days and are shorter in summer and longer in winter. It will also be washed out by rain.

Cleanup/Disposal: Guide No. 127: Eliminate all ignition sources (no smoking, flares, sparks or flames in immediate area). All equipment used when handling the product must be grounded. Do not touch or walk through spilled material. Stop leak if you can do it without risk. Prevent entry into waterways, sewers, basements or confined areas. A vapor suppressing foam may be used to reduce vapors. Absorb or cover with dry earth, sand or other non-combustible material and transfer to containers. Use clean non-sparking tools to collect absorbed material. Large Spills: Dike far ahead of liquid spill for later disposal. Water spray may reduce vapor; but may not prevent ignition in closed spaces.

Environmental Physical Data

Henry's Law Constant: 3.97 x10⁻⁵

Octanol/Water Partition Coefficient: log K_{OW} = -0.24

BCF: negligible

BOD: theoretical 122%, 5 days

Regulations

RCRA 40CFR: Listed Hazardous Waste No. U002 Ignitable Waste

CERCLA: 40CFR 302.4: Listed per RCRA Section 3001 RQ: 5000 lb (2268 kg)

SARA 40CFR 372.65: Not listed

SARA EHS 40CFR 355: Not listed

TSCA: Listed

Analytical Methods

Air: EPA 0100, OA-002-1, VA-005-1, VG-006-1, TO-11, TO-5; ASTM D3686, D3687, D4490

Soil: CLP LC_VOA, MC_VOA, OHC; EPA 1624; SW846 1311, 5031, 5032, 5041, 5041A, 8015B, 8240B, 8260A, 8260B, 8315, 8315A; DOE OG015R

Water / Groundwater: EPA VW-008-1; ASTM D3695, D4763

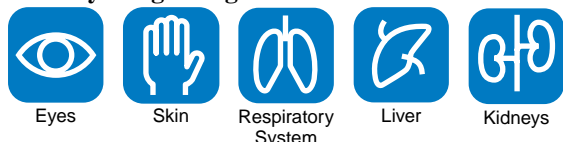
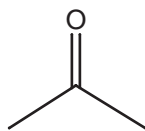
Drinking Water: EPA 524.2

Food: AOAC 975.06

Indoor / Expired Air: NIOSH 1300; EPA IP-6A, IP-6B, IP-6C, 0100

Plasma: EPA 29

Other: EPA VS-006-1

Primary Target Organs:**Environmental****Regulations****RCRA 40CFR:** Not listed**CERCLA: 40CFR 302.4:** Not listed**SARA 40CFR 372.65:** Not listed**SARA EHS 40CFR 355:** Not listed**TSCA:** Listed**ACE4750****CAS #: 67-64-1****ACETONE****RTECS:** AL3150000**DOT:** UN1090; IMO3.1**EINECS Number:** 200-662-2**Molecular Formula:** C₃H₆O**Structured MF:** CH₃COCH₃**Formula Weight:** 58.09**Chemical Structure**

Synonyms: ACETON; CHEVRON ACETONE; DIMETHYL KETONE; DIMETHYLFORMALDEHYDE; DIMETHYLKETAL; EPA PESTICIDE CHEMICAL CODE 004101; KETONE PROPANE; KETONE, DIMETHYL; BETA-KETOPROPANE; METHYL KETONE; 2-PROPANONE; PROPANONE; PYROACETIC ACID; PYROACETIC ETHER

Description: colorless liquid; sweetish odor

Use: in the manufacture of smokeless powder, paints, varnishes, lacquers, organic chemicals, pharmaceuticals, sealants, adhesives, methyl isobutyl ketone, mesityl oxide, acetic acid (ketene process), diacetone alcohol, chloroform, iodoform, bromoform, explosives, airplane dopes, rayon, photographic films, isoprene, methyl isobutyl carbinol, methyl methacrylate and bisphenol A; as solvent for cellulose acetate, nitrocellulose, acetylene, fats, oils, waxes, resins, rubber, plastics, rubber cements, pharmaceuticals, potassium iodide and permanganate; in storing acetylene gas, in purifying paraffin, in hardening and dehydrating tissues an to clean and dry parts of precision equipment; in extraction of various principles from animal and plant substances, as a delusterant for cellulose acetate fibers, in specification testing of vulcanized rubber products, as a cosmetic ingredient, as a dye intermediate and in paint and varnish removers

Physical Properties**Boiling Point:** 56.2 °C (133 °F) at 760 mm Hg**Freezing Point:** -95.35 °C (-139.63 °F)**Specific Gravity:** 0.7899 at 20 °C/4 °C**Vapor Density:** 2 Air=1**Saturated Vapor Density:** 1.565868784 kg/m³**Density:** 0.786 gm/cc at 22.7 °C**Vapor Pressure:** 231 mm Hg at 25 °C**Water Solubility:** Miscible**Other Solubilities:** 95% Ethanol: >=100 mg/ml at 22 °C;

Acetone: >=100 mg/ml at 22 °C; Benzene: Soluble;

Chloroform: miscible; DMSO: >=100 mg/ml at 22 °C; Ether: miscible; Methanol: miscible; Most oils: miscible; Organic solvents: miscible.

Surface Tension: 26.2 nM/M at 0 °C**Odor Threshold:** 47.5 to 1613.9 mg/m³**Refraction Index:** 1.3588 at 20 °C/D**Evaporation Rate:** < 1 Butyl Acetate=1**Critical Temperature:** 235 °C**Critical Pressure:** 46.4 atm**Ionization Potential (eV):** 9.69**Flash Point:** -20 °C**Autoignition Temperature:** 465 °C**LEL:** 2.15% v/v**UEL:** 13% v/v**RTECS Toxicity Data****Acute Oral:** Man TD_{Lo} Dose: 2857 mg/kg; Toxic Effects:Behavioral - Coma; Kidney, Ureter, and Bladder - Other changes. Man TD_{Lo} Dose: 2857 mg/kg; Toxic Effects:Behavioral - Coma; Biochemical - Other. Rat LD₅₀ Dose: 5800 mg/kg; Toxic Effects: Behavioral - Altered sleep time (including change in righting reflex); Behavioral - Tremor.**Acute Inhalation:** Rat LC₅₀ Dose: 50100 mg/m³/8hr. Human TC_{Lo} Dose: 500 ppm; Toxic Effects: Sense organs and special senses - Other; Sense organs and special senses - Conjunctive irritation; Lungs, Thorax, or Respiration - Other changes.Man TC_{Lo} Dose: 440 ug/m³/6M; Toxic Effects: Brain and coverings - Recordings from specific areas of CNS. Man TC_{Lo} Dose: 10 mg/m³/6hr; Toxic Effects: Biochemical - Other carbohydrates. Man TC_{Lo} Dose: 12000 ppm/4hr; Toxic Effects: Gastrointestinal - Nausea or vomiting; Behavioral - Muscle weakness.**Acute Dermal:** Rabbit LD_{Lo} Route: Skin; Dose: 20 mL/kg.Guinea Pig LD₅₀ Route: Skin; Dose: >9400 mg/kg.**Chronic (Multiple Dose) Oral:** Rat Dose: 273 gm/kg/13W-C; Toxic Effects: Liver - Changes in liver weight; Kidney, Ureter, and Bladder - Changes in kidney weight; Blood - Normocytic anemia. Mouse Dose: 546 gm/kg/13W-C; Toxic Effects: Liver - Changes in liver weight; Endocrine - Changes in spleen weight.**Chronic (Multiple Dose) Inhalation:** Rat Dose: 19000 ppm/3H/8W-I; Toxic Effects: Brain and coverings - Changes in brain weight. Rat Dose: 199 mg/m³/8H/45D-I; Toxic Effects: Behavioral - Muscle contraction or spasticity.**Irritation Eye:** Rabbit Standard Draize Test Dose: 20 mg/24H; Reaction: moderate. Rabbit Standard Draize Test Dose: 20 mg; Reaction: severe.**Irritation Skin:** Rabbit Standard Draize Test Dose: 500 mg/24H; Reaction: mild. Rabbit Open Draize Test Dose: 395 mg open; Reaction: mild.

Reproductive/Teratogenic: Rat Route: Oral; Dose: 273 gm/kg; Duration: male 13W prior to mating; Paternal Effects - Spermatogenesis. Mammal Route: Inhalation; Dose: 31500 ug/m³; Duration: female 1-13D of pregnancy; Effects on Fertility - Post-implantation mortality.

Mutagenic: Hamster Cytogenetic Analysis; Cell Type: fibroblast; Dose: 40 gm/L. Yeast - *S Cerevisiae* Sex Chromosome Loss; Dose: 47600 ppm.

Hazard Overviews



Flammable



Fire
Diamond

Health: Irritating to eyes/skin/respiratory tract. Also Causes: muscle weakness, mental confusion, coma (high concentrations) ingestion: GI irritation, kidney and liver damage, metabolic changes, coma. Chronic Effects: dermatitis.

Fire: Flammable. Can form explosive mixtures in the air. Do not extinguish fire unless flow can be stopped. For small fires, use dry chemical, carbon dioxide, water spray or alcohol-resistant foam. For large fires, use water spray, fog, or alcohol-resistant foam. Use water in flooding quantities as fog because solid streams may be ineffective.

Reactivity: Stable. Hazardous polymerization cannot occur. Avoid: contact with plastic eyeglass frames, jewelry, pens, pencils, and rayon garments. Incompatible with: hydrogen peroxide; acetic acid; nitric acid; nitric acid and sulfuric acid; chromic anhydride; chromyl chloride; nitrosyl chloride; hexachloromelamine; nitrosyl perchlorate; nitryl perchlorate; permonosulfuric acid; thiodiglycol and hydrogen peroxide; oxidizing materials; activated carbon; chromium trioxide; dioxygen difluoride and carbon dioxide; potassium-tert-butoxide; air; bromoform; bromine; chloroform and alkalies; trichloromelamine; sulfur dichloride. Hazardous decomposition products: carbon dioxide; carbon monoxide.

Carcinogenicity: IARC - Not listed; NIOSH - Not listed; NTP - Not listed; ACGIH - Not listed; OSHA - Not listed; EPA - Class D, Not classifiable as to human carcinogenicity; MAK - Not listed

Primary Target Organs:



Eyes



Skin



Respiratory
System



Gastro-
intestinal



Nervous
System

Exposure Limits

OSHA PEL: TWA: 1000 ppm; 2400 mg/m³.

OSHA PEL Vacated 1989 Limits: TWA: 750 ppm; 1800 mg/m³; STEL: 1000 ppm; 2400 mg/m³.

ACGIH TLV: TWA: 750 ppm; 1780 mg/m³; STEL: 1000 ppm; 2380 mg/m³.

NIOSH REL: TWA: 250 ppm; 590 mg/m³.

NIOSH IDLH: 2500 ppm; LEL.

DFG MAK: TWA: 500 ppm; 1200 mg/m³.

Respirator Recommendation

Exposure Range: >1000 to <2500 ppm Supplied Air, Constant Flow/Pressure Demand, Full Face

Exposure Range: 2500 to unlimited ppm Self-contained Breathing Apparatus, Pressure Demand, Full Face

Note: use ov (black) cartridge for nuisance (<1000)

Environmental

Ecotoxicity: LD₁₀₀ *Asellus aquaticus* 3 ml/l (within 3 days of exposure) /Conditions of bioassay not specified LC₅₀ Mexican axolotl 20.0 mg/l/48 hr (3-4 weeks after hatching) /Conditions of bioassay not specified TLM Mosquito fish 13,000 mg/l/24, 48, 96 hr /Conditions of bioassay not specified LD₁₀₀ *Gammarus fossarum* 10 ml/l (within 48 hr) /Conditions of bioassay not specified LC₅₀ *Poecilia reticulata* (guppy) 7,032 ppm/14 days /Conditions of bioassay not specified LC₅₀ Ring-necked pheasant oral greater than 40,000 ppm, in diet, age 10 days, (no mortality to 40,000 ppm) LC₅₀ *Salmo gairdneri* (Rainbow trout) 5,540 mg/l/96 hr at 12 °C (95% confidence limit 4,740-6,330 mg/l), wt 1.0 g /static bioassay LC₅₀ Clawed toad 24.0 mg/l/48 hr (3-4 weeks after hatching) /Conditions of bioassay not specified TLM *Daphnia magna* 10 mg/l/24, 48 hr /Conditions of bioassay not specified

Environmental Fate: If released on soil, it will both volatilize and leach into the ground and probably biodegrade. If released into water, it will probably biodegrade. It will also be lost due to volatilization (estimated half-life 20 hr from a model river). Bioconcentration in aquatic organisms and adsorption to sediment should not be significant. In the atmosphere, it will be lost by photolysis and reaction with photochemically produced hydroxyl radicals. Half-life estimates from these combined processes average 22 days and are shorter in summer and longer in winter. It will also be washed out by rain.

Cleanup/Disposal: Guide No. 127: Eliminate all ignition sources (no smoking, flares, sparks or flames in immediate area). All equipment used when handling the product must be grounded. Do not touch or walk through spilled material. Stop leak if you can do it without risk. Prevent entry into waterways, sewers, basements or confined areas. A vapor suppressing foam may be used to reduce vapors. Absorb or cover with dry earth, sand or other non-combustible material and transfer to containers. Use clean non-sparking tools to collect absorbed material. Large Spills: Dike far ahead of liquid spill for later disposal. Water spray may reduce vapor; but may not prevent ignition in closed spaces.

Environmental Physical Data

Henry's Law Constant: 3.97 x 10⁻⁵

Octanol/Water Partition Coefficient: log K_{ow} = -0.24

BCF: negligible

BOD: theoretical 122%, 5 days

Regulations

RCRA 40CFR: Listed Hazardous Waste No. U002 Ignitable Waste

CERCLA: 40CFR 302.4: Listed per RCRA Section 3001 RQ: 5000 lb (2268 kg)

SARA 40CFR 372.65: Not listed
SARA EHS 40CFR 355: Not listed
TSCA: Listed

Analytical Methods

Air: EPA 0100, OA-002-1, VA-005-1, VG-006-1, TO-11, TO-5; ASTM D3686, D3687, D4490

Soil: CLP LC_VOA, MC_VOA, OHC; EPA 1624; SW846 1311, 5031, 5032, 5041, 5041A, 8015B, 8240B, 8260A, 8260B, 8315, 8315A; DOE OG015R

Water / Groundwater: EPA VW-008-1; ASTM D3695, D4763

Drinking Water: EPA 524.2

Food: AOAC 975.06

Indoor / Expired Air: NIOSH 1300; EPA IP-6A, IP-6B, IP-6C, 0100

Plasma: EPA 29

Other: EPA VS-006-1

ACE4900 CAS #: 1752-30-3

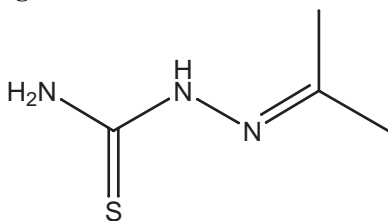
ACETONE THIOSEMICARBAZIDE

RTECS: AL7350000

EINECS Number: 217-137-9

Molecular Formula: C₄H₉N₃S

Formula Weight: 131.22



Chemical Structure

Synonyms: ACETONE THIOSEMICARBAZONE;
 ACETONTHIOSEMIKARBAZON; HYDRAZINECARBOTHIOAMIDE,2-(1-METHYLETHYLIDENE)-; HYDRAZINECARBOTHIOAMIDE,2-(1-METHYLETHYLIDENE)-(9CI); 2-(1-METHYLETHYLIDENE)HYDRAZINECARBOTHIOAMIDE;
 THIOSEMICARBAZONE ACETONE

Description: white, needle-shaped crystalline powder; odorless

RTECS Toxicity Data

Acute Oral: Rat LD₅₀ Dose: 10 mg/kg.

Hazard Overviews

Carcinogenicity: IARC - Not listed; NIOSH - Not listed; NTP - Not listed; ACGIH - Not listed; OSHA - Not listed; EPA - Not listed; MAK - Not listed

Environmental

Regulations

RCRA 40CFR: Not listed

CERCLA: 40CFR 302.4: Not listed

SARA 40CFR 372.65: Not listed TPQ: 1000/10000 lb
SARA EHS 40CFR 355: Listed TPQ: 1000 lb
TSCA: Listed

ACE5050

CAS #: 75-05-8

ACETONITRILE

RTECS: AL7700000

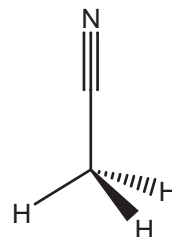
DOT: UN1648; IMO3.2

EINECS Number: 200-835-2

Molecular Formula: C₂H₃N

Structured MF: CH₃CN

Formula Weight: 41.05



Chemical Structure

Synonyms: ACETONITRIL; CYANOMETHANE; CYANURE DE METHYL; ETHANENITRILE; ETHYL NITRILE; METHANECARBONITRILE; METHANE,CYANO-; METHYL CYANIDE; METHYLKYANID

Description: clear, colorless liquid; aromatic odor

Use: chemical intermediate in the synthesis of acetophenone, 1-naphthaleneacetic acid, thiamine and acetamidine, in pesticide manufacture, as an extractant for animal and vegetable oils, as a pharmaceutical solvent, as a solvent for inorganic salts and in organic synthesis, as a polymer solvent and in acrylic fibers; for separation of butadiene by extractive distillation, in perfumes, in nitrile rubber, in ABS resins, as a solvent in hydrocarbon extraction processes, as a specialty solvent, as a catalyst, to remove tars, phenols and coloring matter from petroleum hydrocarbons which are not soluble in acetonitrile, to recrystallize steroids, as an indifferent medium in physicochemical investigations, as a medium for promoting reactions involving ionizations and as a solvent in non-aqueous titrations

Physical Properties

Boiling Point: 81.6 °C (179 °F) at 760 mm Hg

Freezing Point: -45 °C (-49 °F)

Specific Gravity: 0.78745 at 15 °C/4 °C

Vapor Density: 1.42 Air=1

Saturated Vapor Density: 1.257078947 kg/m³

Density: 0.7857 g/mL at 20 °C

Vapor Pressure: 87 mm Hg at 24 °C

Water Solubility: Miscible with Water

Other Solubilities: Equal wt of acetonitrile and the following materials are miscible at room temp: formic acid, Acetic Acid, Methanol, cellosolve solvent, formaldehyde,