

CAS 108-01-0 2-Dimethylaminoethanol DMEA

2-Dimethylaminoethanol

CAS No.108-01-0

Chemical Name:2-Dimethylaminoethanol Synonyms

DMAE;DMEA;DIMETHYLAMINOETHANOL;N,N-

DIMETHYLETHANOLAMINE;DIMETHYLETHANOLAMINE;DEANOL;2-(N,N-

DIMETHYLAMINO)ETHANOL;N,N-

DIMETHYLAMINOETHANOL;DMEOA;DIMETHYL MEA



CBNumber:CB6256870

Molecular Formula:C₄H₁₁NO

Molecular Weight:89.14

MDL Number:MFCD00002846

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Brand Designation / Product Code Table

Brand / Manufacturer	Product Grade / Code	Notes
Dabco (Evonik / ex-Air Products)	Dabco DMEA	Industry standard naming
Jeffcat (Huntsman)	Jeffcat DMEA	Direct product designation
KAOLIZER (Kao Corporation)	KAOLIZER No. 25	Kao's numeric amine designation (No. 10 is <i>DMCHA</i> , No. 25 is <i>DMEA</i>)
Lupragen (BASF)	Lupragen N101	BASF standard designation
Polycat (Evonik)	Polycat DMEA	Direct commodity designation
Tegoamin (Evonik)	Tegoamin DMEA	Evonik flexible/specialty foam catalyst line
Toyocat (Tosoh)	Toyocat-DMA (or Toyocat DMEA)	Tosoh amine catalyst line
FASCAT (PMC Organometallics)	N/A (Not Applicable)	FASCAT is exclusively reserved for organometallic catalysts (tin, bismuth, titanium, etc.), not pure tertiary amines like DMEA.
U-CAT (San-Apro)	U-CAT DMEA	San-Apro organic amine series

2-Dimethylaminoethanol Properties

Melting point −70 °C(lit.)

Boiling point 134-136 °C(lit.)

Density 0.886 g/mL at 20 °C(lit.)

vapor density 3.03 (vs air)

vapor pressure 100 mm Hg (55 °C)

refractive index $n_{20/D}$ 1.4294(lit.)

Flash point 105 °F

storage temp. Store below +30°C.

solubility alcohol: miscible(lit.)

form Liquid

pKa pK_1 :9.26(+1) (25°C)

color Clear colorless to pale yellow

Odor Amine like

PH Range 10.5 - 11.0 at 100 g/l at 20 °C

PH 10.5-11 (100g/l, H₂O, 20°C)

explosive limit 1.4-12.2%(V)

Water Solubility miscible

FreezingPoint -59.0°C

Sensitive Hygroscopic

Merck 14,2843

BRN 1209235

Henry's Law Constant 9.3×10^1 mol/(m³Pa) at 25°C, Nguyen (2013)

Stability Stable. Flammable. Incompatible with oxidizing agents, copper, copper alloys, zinc, acids, galvanised iron. Hygroscopic.

Cosmetics Ingredients Functions BUFFERING

InChI 1S/C4H11NO/c1-5(2)3-4-6/h6H,3-4H2,1-2H3

InChIKey UEEJHVSXFDXPFK-UHFFFAOYSA-N

SMILES CN(C)CCO

LogP -0.55 at 23°C

Substances Added to Food (formerly EAFUS) DIMETHYLETHANOLAMINE

FDA 21 CFR 173.20; 175.105; 175.300

SAFETY

Signal word Danger

Hazard statements H331-H302+H312-H314-H335-H226

Precautionary statements P501-P270-P240-P261-P210-P233-P243-P241-P242-P271-P264-P280-P370+P378-P362+P364-P303+P361+P353-P301+P330+P331-P301+P312+P330-P304+P340+P310-P305+P351+P338+P310-P403+P233-P403+P235-P405

target organs Respiratory system

PPE Faceshields, Gloves, Goggles, type ABEK (EN14387) respirator filter
Hazard Codes C
Risk Statements 10-20/21/22-34
Safety Statements 25-26-36/37/39-45
RIDADR UN 2051
WGK Germany 1
RTECS KK6125000
Autoignition Temperature 245 °C
TSCA TSCA listed
Hazard Class 8
Packing Group II
HS Code 29221980
Storage Class 3 - Flammable liquids
Hazard Classifications Acute Tox. 3 Inhalation
Acute Tox. 4 Dermal
Acute Tox. 4 Oral
Eye Dam. 1
Flam. Liq. 3
Skin Corr. 1B
STOT SE 3
Hazardous Substances Data 108-01-0 (Hazardous Substances Data)
Toxicity LD50 orally in Rabbit: 2130 mg/kg LD50 dermal Rabbit 1220 mg/kg
REACH Registrations Active
Limited Quantities 1.0 L (0.3 gallons) (liquid) or 1 Kg (2.2 lbs) (solid)
Excepted Quantities Max Inner Pack (30g or 30ml) and Max Outer Pack (500g or 500ml)

2-Dimethylaminoethanol Chemical Properties, Uses, Production

Description

Dimethylaminoethanol is a colorless liquid with a pungent odor. Odor threshold: 0.25 ppm. Molecular weight 59.16; Boiling point = 133 °C; Freezing/Melting point = -25.9 °C; Flash point = 41 °C (OC); Autoignition temperature = 295 °C. Explosive limits: LEL = 1.6%; UEL = 11.9%. Hazard Identification (based on NFPA-704M Rating System): Health 2, Flammability 2, Reactivity 0. Soluble in water.

Chemical Properties

colorless or slightly yellow liquid with ammonia odor. It is miscible with water, ethanol, benzene, ether and acetone.

Uses

dimethyl MEA (DMAE) is also known as dimethylaminoethanol. Studies indicate skin-firming properties, and an ability to reduce the appearance of fine lines and wrinkles as well as dark circles under the eyes. It is considered anti-aging, and antiinflammatory, and has exhibited free-radical scavenging activity.

Uses

2-(Dimethylamino)ethanol is used as corrosion inhibitor, anti-scaling agent, paint additive, coating additive and solids separation agent. It is also used as an intermediate for active pharmaceutical ingredients and dyes. It serves as a curing agent for polyurethanes and epoxy resins. Further, it is used as an additive to boiler water. In addition to this, it is used therapeutically as a CNS stimulant.

Uses

2-Dimethylaminoethanol (deanol, DMAE) may be employed as a ligand in the copper-catalyzed amination of aryl bromides and iodides.

Preparation

The synthesis of 2-Dimethylaminoethanol by the ethylene oxide method is obtained by the ammonification of dimethylamine with ethylene oxide, which is distilled, refined and dehydrated.

Definition

ChEBI: N,N-dimethylethanolamine is a tertiary amine that is ethanolamine having two N-methyl substituents. It has a role as a curing agent and a radical scavenger. It is a tertiary amine and a member of ethanolamines.

Production Methods

Synthesis of dimethylaminoethanol can be accomplished from equimolar amounts of ethylene oxide and dimethylamine (HSDB 1988).

General Description

A clear colorless liquid with a fishlike odor. Flash point 105°F. Less dense than water. Vapors heavier than air. Toxic oxides of nitrogen produced during combustion. Used to make other chemicals.

Air & Water Reactions

Flammable. Partially soluble in water and less dense than water.

Reactivity Profile

DIMETHYLAMINOETHANOL is an aminoalcohol. Amines are chemical bases. They neutralize acids to form salts plus water. These acid-base reactions are exothermic. The amount of heat that is evolved per mole of amine in a neutralization is largely independent of the strength of the amine as a base. Amines may be incompatible with isocyanates, halogenated organics, peroxides, phenols (acidic), epoxides, anhydrides, and acid halides. Flammable gaseous hydrogen is generated by amines in combination with strong reducing agents, such as hydrides. N,N-Dimethylethanolamine may react vigorously with oxidizing materials.

Health Hazard

Dimethylaminoethanol is classified as a mild skin irritant and a severe eye irritant (HSDB 1988). Doses as high as 1200 mg daily produce no serious side effects and a single dose of 2500 mg taken in a suicide attempt had no adverse effects (Gosselin et al 1976). Inhalation of the vapor or mist can cause irritation to the upper respiratory tract. Asthmatic symptoms have been reported. Extremely irritating; may cause permanent eye injury. Corrosive; will cause severe skin damage with burns and blistering. Ingestion may cause damage to the mucous membranes and gastrointestinal tract. No reports were found in the literature regarding carcinogenic or mutagenic potential.

Flammability and Explosibility

Flammable

Industrial uses

Dimethylaminoethanol is used as a chemical intermediate for antihistamines and local anesthetics; as a catalyst for curing epoxy resins and polyurethanes; and as a pH

control agent for boiler water treatment. However, dimethylaminoethanol in the salt form, (i.e. dimethylaminoethanol acetamidobenzoate) is primarily utilized therapeutically as an antidepressant (HSDB 1988).

Safety Profile

Moderately toxic by ingestion, inhalation, skin contact, intraperitoneal, and subcutaneous routes. A skin and severe eye irritant. Used medically as a central nervous system stimulant. Flammable liquid when exposed to heat or flame; can react vigorously with oxidizing materials. Ignites spontaneously in contact with cellulose nitrate of high surface area. To fight fire, use alcohol foam, foam, CO₂, dry chemical. When heated to decomposition it emits toxic fumes of NO_x

Potential Exposure

Primary Irritant. Dimethylaminoethanol is used as a corrosion inhibitor; pharmaceutical intermediate; in making dyestuffs, textiles, pharmaceuticals; emulsifiers in paints and coatings. Also, it has been used as a medication in the treatment of behavioral problems of children.

First aid

If this chemical gets into the eyes, remove any contact lenses at once and irrigate immediately for at least 15 min, occasionally lifting upper and lower lids. Seek medical attention immediately. If this chemical contacts the skin, remove contaminated clothing and wash immediately with soap and water. Seek medical attention immediately. If this chemical has been inhaled, remove from exposure, begin rescue breathing (using universal precautions, including resuscitation mask) if breathing has stopped and CPR if heart action has stopped. Transfer promptly to a medical facility. When this chemical has been swallowed, get medical attention. If victim is conscious, administer water or milk. Do not induce vomiting. Medical observation is recommended for 24—48 h after breathing overexposure, as pulmonary edema may be delayed. As first aid for pulmonary edema, a doctor or authorized paramedic may consider administering a corticosteroid spray.

Metabolism

When administered orally, dimethylaminoethanol acetamidobenzoate (the therapeutic salt formulation) has been shown to cross the blood-brain barrier (HSDB 1988). Two

other studies have examined the pharmacokinetics of dimethylaminoethanol in rats (Dormand et al 1975) and healthy adults (Bismut et al 1986).

It has been postulated that dimethylaminoethanol undergoes endogenous methylation (LaDu et al 1971). After intravenous treatment of mice with [14C]-labeled dimethylaminoethanol in the brain, dimethylaminoethanol yielded phosphoryldimethylaminoethanol and phosphatidyl dimethylaminoethanol. Acid-soluble and lipid cholines derived from dimethylaminoethanol also were found in brain (Miyazaki et al 1976). While examining the pharmacokinetics of the maleate acid of [14C]-dimethylaminoethanol in rats, Dormand et al (1975) observed that dimethylaminoethanol was metabolized in the phospholipid cycle and produced metabolites such as phosphoryldimethylaminoethanolamine, and glycerophosphatidylcholine. In kainic-acid lesioned rats, dimethylaminoethanol was converted to a substance which cross-reacted in the radioenzymatic assay for acetylcholine (London et al 1978). Ansell and Spanner (1979) demonstrated that [14C]-dimethylaminoethanol rapidly disappeared from brain; after 0.5, 1, and 7 h, only 30, 27, and 16% of the administered radioactivity, respectively, remained in the brain after intracerebral injection. They also showed that brain levels of phosphodimethylaminoethanol increased to a maximum at 1-2 h and decreased afterwards, whereas concentrations of phosphatidylethanolamine increased continuously throughout the 7 h observation period. This study further found that after i.p. injections of labeled dimethylaminoethanol, the brain content of phosphatidylethanolamine increased through the 7 h period and the levels were 10-40 fold higher than those of phosphodimethylaminoethanol.

Shipping

Label of "CORROSIVE, FLAMMABLE LIQUID." It falls in Hazard Class 8. Packing Group II. Spill Handling: Evacuate and restrict persons not wearing protective equipment from area of spill or leak until cleanup is complete. Remove all ignition sources. Establish forced ventilation to keep levels below explosive limit.

Absorb liquids in vermiculite, dry sand, earth, peat, carbon, or a similar material and deposit in sealed containers. Keep this chemical out of a confined space, such as a sewer, because of the possibility of an explosion, unless the sewer is designed to prevent the buildup of explosive concentrations. It may be necessary to contain and dispose of this chemical as a hazardous waste. If material or contaminated runoff enters waterways, notify downstream users of potentially contaminated waters. Contact your

local or federal environmental protection agency for specific recommendations. If employees are required to clean up spills, they must be properly trained and equipped. OSHA 1910.120(q) may be applicable.

Purification Methods

Dry the amine with anhydrous K_2CO_3 or KOH, and fractionally distil it. [Beilstein 4 IV 1424.]

Incompatibilities

Forms explosive mixture with air. Violent reaction with oxidizers, strong acids, acid chlorides, and isocyanates. Attacks copper and its alloys, galvanized steel, zinc and its alloys.

Toxics Screening Level

The initial threshold screening level (ITSL) for dimethylethanolamine (CAS #108-01-0) is 5.2 $\mu\text{g}/\text{m}^3$ with an annual averaging time and a second ITSL for dimethylethanolamine is 220 $\mu\text{g}/\text{m}^3$ with an 8-hour averaging time.

2-Dimethylaminoethanol Preparation Products And Raw materials

Raw materials

ETHYLENE OXIDE 2-Chloroethanol Dimethylamine

Preparation Products

5-Fluoro-2-picolinic acid PROPIONYLTHIOCHOLINE IODIDE 1-[6-(Trifluoromethyl)pyridin-2-yl]piperazine polyurethane adhesive 691 Acetylthiocholine iodide 2-Dimethylaminoethyl chloride hydrochloride 4-(2-(DIMETHYLAMINO)ETHOXY)-3,5-DICHLOROBENZENAMINE 2-DIMETHYLAMINOETHANETHIOL HYDROCHLORIDE 2-Chloro-6-trifluoromethylnicotinic acid N,N-Dimethylethylenediamine DOWEX(R) 1X8 S-Butyrylthiocholine Iodide 1-(2-DIMETHYLAMINOETHYL)PIPERAZINE 2-Trifluoromethyl-6-pyridinecarboxylic acid N,N-Dimethyltryptamine Meclofenoxate hydrochloride 2-(Dimethylamino)ethyl (4-chlorophenoxy)acetate 2-bromoethyldimethylamine 2-Chloro-3,6-dimethylpyridine

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