Dimethylamine c2h7n structure

Contents

- Retention Index (Linear):

Molecular Formula	C_2H_7N
Average mass	45. 084 Da
Density	0. 6±0. 1 g/cm ^{3}
Boiling Point	6. 1±3. 0 °C at 760 mmHg
Flash Point	-56. 1±8. 8 °C
Molar Refractivity	14. 9±0. 3 cm ^{3}
Polarizability	5. 9±0. 5 10^{-24} cm ^{3}
Surface Tension	15. 5±3. 0 dyne/cm
Molar Volume	70. 4±3. 0 cm ^{3}

- Experimental data
- Predicted – ACD/Labs
- Predicted – EPISuite

- Predicted – ChemAxon
- Experimental Physico-chemical Properties

Experimental Melting Point:

-92 °COxford University

Chemical Safety Data

(No longer

updated)More details

-92 °CJean-Claude

Bradley Open Melting

Point Dataset13102,

16011

-92. 2 °CJean-Claude

Bradley Open Melting

Point Dataset22407

-37 °CSynQuest66318,

3131-1-X3

-93

°CLabNetworkLN00164

054

-96

°CFooDBFDB012589

- **Experimental Boiling Point:**

  44 F (6. 6667

  °C)NIOSHIP8750000

  7. 4 °COxford

  University Chemical

  Safety Data (No longer

  updated)More details

  60 °CAlfa AesarH27665

  52 °CSynQuest66318,

  3131-1-X3

  60

  °COakwood[051280]

  60

  °CLabNetworkLN00164

  054

  7 °CFooDBFDB012589

- **Experimental Ionization Potent:**

  8. 24

  EvNIOSHIP8750000

- **Experimental Vapor Pressure:**

  1. 7 atm (1292

  mmHg)NIOSHIP8750000

- **Experimental LogP:**

  -0. 38Egon

  Willighagenhttp://dx.

  doi. org/10.

  1021/ci050282s

- **Experimental Flash Point:**

  20 F (-6. 6667 °C)(Gas,

  Liquid,

  None)NIOSHIP8750000

  -6 °COxford University

  Chemical Safety Data

  (No longer

  updated)More details

  5 °CAlfa Aesar

  -36 °CAlfa Aesar

  15 °CAlfa Aesar

  5 °F (-15 °C)Alfa

AesarH27261

15 °F (-9. 4444 °C)Alfa

Aesar43261, 31458

-36 °F (-37. 7778

°C)Alfa AesarH27665

16 °CSynQuest66318,

3131-1-X3

16

°COakwood[044754]

-36

°COakwood[051280]

-36

°CLabNetworkLN00164

054

- **Experimental Freezing Point:**

  -134 F (-92. 2222

  °C)NIOSHIP8750000

- **Experimental Gravity:**

  0. 775 g/mLAlfa

AesarH27261

0. 89 g/mLAlfa Aesar43261,

31458

0. 85 g/mLAlfa AesarH27665

0. 89 g/mLSynQuest3131-1-

X3

0. 89 g/mLOakwood[044754]

0. 85 g/mLOakwood[051280]

0. 89

g/mLFluorochem044754

0. 85 g/mLFluorochem

0. 775 g/lFluorochem044754

0. 85 g/lFluorochem051280

- **Experimental Refraction Index:**

1. 37Alfa Aesar43261,

31458

1. 37SynQuest66318,

3131-1-X3

- Miscellaneous

Appearance:

Colorless gas with an ammonia- or fish-like odor. [Note: A liquid below 44F. Shipped as a liquefied compressed gas.]NIOSHIP8750000

colourless gas with strong ammonia-like smellOxford University Chemical Safety Data (No longer updated)More details

Stability:

Stable. Generally used as a solution in water at concentrationsup to around 40%. Extremely flammable in the pure form. Incompatible with strongoxidizing agents. Oxford University Chemical Safety Data

(No longer

updated)More details

- **Toxicity:**

  ORL-RAT LD50 698 mg

  kg-1, ORL-GPG LD50

  240 mg kg-1, IPR-MUS

  LD50 736 mg kg-1,

  ORL-RBT LD50 240 mg

  kg-1Oxford University

  Chemical Safety Data

  (No longer

  updated)More details

- **Safety:**

  11-19-36/37Alfa

  AesarH27665

  11-20-37/38-41Alfa

  Aesar31458, 43261

  11-23/24/25-37/38-

  39/23/24/25-41Alfa

  AesarH27261

  3Alfa Aesar31458,

  43261, H27261,

H27665

4-9-16-20-23-26-27-33-

36/37/39-45-60Alfa

AesarH27261

9-16-23-26-33-39-

60Alfa AesarH27665

9-16-23-26-

36/37/39Alfa

Aesar31458, 43261

DangerAlfa

Aesar31458, 43261,

H27261, H27665

DANGER: FLAMMABLE,

CORROSIVE, burns skin

and eyesAlfa

Aesar31458, 43261

H225-H311-H331-

H370-H314Alfa

AesarH27261

H225-H314-H351-

H335-H336-

EUH019Alfa

AesarH27665

H225-H331-H318-

H302-H315-H335Alfa

Aesar31458, 43261

Highly

Flammable/Corrosive/H

ygroscopicSynQuest31

31-1-X3, 66318

P210-P260-

P303+P361+P353-

P305+P351+P338-

P405-P501aAlfa

AesarH27665

P210-P261-

P303+P361+P353-

P305+P351+P338-

P405-P501aAlfa

Aesar31458, 43261

P210-

P303+P361+P353-

P305+P351+P338-

P361-P405-P501aAlfa

AesarH27261

Safety glasses, gloves,

good ventilation.

Oxford University

Chemical Safety Data

(No longer

updated)More details

- **First-Aid:**

  Eye: Irrigate

  immediately

  (liquid)/Frostbite Skin:

  Water flush

  immediately

  (liquid)/Frostbite

  Breathing: Respiratory

  supportNIOSHIP875000

  0

- **Exposure Routes:**

  inhalation, skin and/or

  eye contact

  (liquid)NIOSHIP875000

  0

- **Symptoms:**

  Irritation nose, throat; sneezing, cough, dyspnea (breathing difficulty); pulmonary edema; conjunctivitis; dermatitis; liquid: frostbiteNIOSHIP8750000

- **Target Organs:**

  Eyes, skin, respiratory systemNIOSHIP8750000

- **Incompatibility:**

  Strong oxidizers, chlorine, mercury, acraldehyde, fluorides, maleic anhydride, aluminum, brass, copper, zincNIOSHIP8750000

- **Personal Protection:**

  Skin: Prevent skin contact (liquid)/Frostbite Eyes: Prevent eye contact (liquid)/Frostbite Wash skin: When contaminated (liquid) Remove: When wet (flammable) Change: No recommendation Provide: Eyewash(liquid), Quick drench (liquid), Frostbite washNIOSHIP8750000

- **Exposure Limits:**

  NIOSH REL : TWA 10 ppm (18 mg/m 3) OSHA PEL : TWA 10 ppm (18 mg/m 3)NIOSHIP8750000

- Gas Chromatography

- **Retention Index (Kovats):**

  419 (estimated with error: 83)NIST Spectramainlib_291481, replib_158546, replib_229435

  405 (Program type: Isothermal; Col… (show more)umn class: Semi-standard non-polar; Column length: 2. 7 m; Column type: Packed; Start T: 100 C; CAS no: 124403; Active phase: Apiezon L; Carrier gas: N2; Substrate: Chromosorb GAW; Data type: Kovats RI; Authors: Golovnya, R. V.; Zhuravleva, N. L.; Svetlova, N. I.; Grigor’eva, D. N., Gas-chromatographic separation of secondary normal

alphatic amines, J.
Anal. Chem. USSR
(Engl. Transl.), 35(10),
1980, 1280-1285, In
original 1976-
1981.)NIST Spectranist
ri

434 (Program type:
Isothermal; Col… (show
more)umn class: Semi-
standard non-polar;
Column type: Packed;
Start T: 100 C; CAS no:
124403; Active phase:
Apiezon L; Data type:
Kovats RI; Authors:
Golovnya, R. V.;
Zhuravleva, I. L., Gas
Chromatographic
Method of Identification
of n-Aliphatic Amines
Through the Use of
Donor-Acceptor
Interaction with
Phosphate,

Chromatographia,

6(12), 1973, 508-

513.)NIST Spectranist ri

458 (Program type:

Isothermal; Col… (show

more)umn class: Semi-

standard non-polar;

Column length: 2. 26

m; Column type:

Packed; Start T: 130 C;

CAS no: 124403; Active

phase: Apiezon L;

Substrate: Teflon-

Haloport; Data type:

Kovats RI; Authors:

Landault, C.; Guiochon,

G., Separation des

amines par

chromatographie gaz-

liquide en utilisant le

teflon comme support,

J. Chromatogr., 13,

1964, 327-336.)NIST

Spectranist ri

646 (Program type: Isothermal; Col… (show more)umn class: Standard polar; Column length: 3 m; Column type: Packed; Start T: 179 C; CAS no: 124403; Active phase: PEG-2000; Carrier gas: He; Substrate: Celite 545 (44-60 mesh); Data type: Kovats RI; Authors: Anderson, A.; Jurel, S.; Shymanska, M.; Golender, L., Gas-liquid chromatography of some aliphatic and heterocyclic mono- and pollyfunctional amines. VII. Retention indices of amines in some polar and unpolar stationary phases, Latv. PSR Zinat. Akad. Vestis Kim. Ser., , 1973, 51-

63.)NIST Spectranist ri

650 (Program type: Isothermal; Col… (show more)umn class: Standard polar; Column length: 3 m; Column type: Packed; Start T: 152 C; CAS no: 124403; Active phase: PEG-2000; Carrier gas: He; Substrate: Celite 545 (44-60 mesh); Data type: Kovats RI; Authors: Anderson, A.; Jurel, S.; Shymanska, M.; Golender, L., Gas-liquid chromatography of some aliphatic and heterocyclic mono- and pollyfunctional amines. VII. Retention indices of amines in some polar and unpolar stationary phases, Latv. PSR Zinat. Akad. Vestis Kim.

Ser., , 1973, 51-

63.)NIST Spectranist ri

- **Retention Index (Normal Alkane):**

  434 (Program type:

  Ramp; Column cl…

  (show more)ass:

  Standard non-polar;

  Column type: Capillary;

  CAS no: 124403; Active

  phase: Methyl Silicone;

  Data type: Normal

  alkane RI; Authors:

  Chen, Y.; Feng, C.,

  QSPR study on gas

  chromatography

  retention index of

  some organic

  pollutants, Comput.

  Appl. Chem. (China),

  24(10), 2007, 1404-

  1408.)NIST Spectranist

  ri

  425 (Program type:

  Ramp; Column cl…

(show more)ass:

Standard non-polar;

Column diameter: 0. 20

mm; Column length: 25

m; Column type:

Capillary; Heat rate: 6

K/min; Start T: 50 C;

End T: 250 C; CAS no:

124403; Active phase:

OV-101; Carrier gas:

N2/He; Phase

thickness: 0. 10 um;

Data type: Normal

alkane RI; Authors:

Zenkevich, I. G.,

Experimentally

measured retention

indices., 2005.)NIST

Spectranist ri

- **Retention Index (Linear):**

426 (Program type:

Ramp; Column cl…

(show more)ass: Semi-

standard non-polar;

Column diameter: 0. 25

mm; Column length: 30 m; Column type: Capillary; Heat rate: 3 K/min; Start T: 60 C; End T: 240 C; CAS no: 124403; Active phase: DB-5; Carrier gas: He; Phase thickness: 0. 25 um; Data type: Linear RI; Authors: Flamini, G.; Luigi Cioni, P.; Morelli, I., Volatiles from leaves, fruits, and virgin oil from Olea europaea Cv. Olivastra Seggianese from Italy, J. Agric. Food Chem., 51, 2003, 1382-1386.)NIST Spectranist ri

Predicted data is generated using the ACD/Labs Percepta Platform – PhysChem Module

Density:	0. 6±0. 1 g/cm ^{3}
Boiling Point:	6. 1±3. 0 °C at 760 mmHg

Vapour Pressure:	1520. 3±0. 0 mmHg at 25°C
Enthalpy of Vaporization:	26. 4±0. 0 kJ/mol
Flash Point:	-56. 1±8. 8 °C
Index of Refraction:	1. 344
Molar Refractivity:	14. 9±0. 3 cm^3
#H bond acceptors:	1
#H bond donors:	1
#Freely Rotating Bonds:	0
#Rule of 5 Violations:	0
ACD/LogP:	-0. 43
ACD/LogD (pH 5. 5):	-3. 38
ACD/BCF (pH 5. 5):	1. 00
ACD/KOC (pH 5. 5):	1. 00
ACD/LogD (pH 7. 4):	-3. 18
ACD/BCF (pH 7. 4):	1. 00

ACD/KOC (pH 7. 4):	1. 00
Polar Surface Area:	12 Å ^{2}
Polarizability:	5. 9±0. 5 10 $^{-24}$ cm ^{3}
Surface Tension:	15. 5±3. 0 dyne/cm
Molar Volume:	70. 4±3. 0 cm ^{3}

Predicted data is generated using the US Environmental Protection Agency's EPISuite™

Log Octanol-Water Partition Coef (SRC): Log Kow (KOWWIN v1. 67 estimate) = -0. 17Log Kow (Exper. database match) = -0. 38Exper. Ref: Hansch, C et al. (1995)Boiling Pt, Melting Pt, Vapor Pressure Estimations (MPBPWIN v1. 42): Boiling Pt (deg C): 16. 06 (Adapted Stein & Brown method)Melting Pt (deg C): -106. 24 (Mean or Weighted MP)VP(mm Hg, 25 deg C): 1. 47E+003 (Mean VP of Antoine & Grain methods)MP (exp database): -92. 2 deg CBP (exp database): 6. 8 deg CVP (exp database): 1. 52E+03 mm Hg at 25 deg CWater Solubility Estimate from Log Kow (WSKOW v1. 41): Water Solubility at 25 deg C (mg/L): 1e+006log Kow used: -0. 38 (expkow database)no-melting pt equation usedWater Sol (Exper. database match) = 1. 63e+006 mg/L (40 deg C)Exper. Ref: SCHWEIZER, AE ET AL. (1978)Water Sol Estimate from Fragments: Wat Sol (v1. 01 est) = 1e+006 mg/LWat Sol (Exper. database match) = 1630000. 00Exper. Ref: SCHWEIZER, AE ET AL. (1978)ECOSAR Class Program (ECOSAR v0. 99h): Class(es) found: Aliphatic AminesHenrys Law Constant (25 deg C) [HENRYWIN v3. 10]: Bond Method : 1. 66E-005 atm-m3/moleGroup Method: 1. 81E-005 atm-m3/moleExper Database: 1. 77E-05 atm-m3/moleHenrys LC [VP/WSol estimate using EPI values]: 4. 508E-005 atm-m3/moleLog Octanol-Air Partition Coefficient (25 deg C) [KOAWIN v1. 10]: Log Kow used: -0. 38 (exp database)Log Kaw used: -3. 140 (exp database)Log Koa (KOAWIN v1. 10 estimate): 2. 760Log Koa (experimental database): 2. 000Probability of Rapid Biodegradation (BIOWIN v4. 10): Biowin1 (Linear Model) : 0. 8799Biowin2 (Non-Linear Model) : 0. 9701Expert Survey Biodegradation Results: Biowin3 (Ultimate Survey Model): 3. 1240 (weeks)Biowin4 (Primary Survey Model) : 3. 8260 (days)MITI Biodegradation Probability: Biowin5 (MITI Linear Model) : 0. 6121Biowin6 (MITI Non-Linear Model): 0. 7268Anaerobic Biodegradation Probability: Biowin7 (Anaerobic Linear Model): 0. 8542Ready Biodegradability Prediction: YESHydrocarbon Biodegradation (BioHCwin v1. 01): Structure incompatible with current estimation method! Sorption to aerosols (25 Dec C)[AEROWIN v1. 00]: Vapor pressure (liquid/subcooled): 2. 03E+005 Pa (1. 52E+003 mm Hg)Log Koa (Exp database): 2. 000Kp (particle/gas partition coef. (m3/ug)): Mackay model : 1. 48E-011 Octanol/air (Koa) model: 2. 45E-011 Fraction sorbed to airborne particulates (phi): Junge-Pankow model : 5. 35E-010 Mackay model : 1. 18E-009 Octanol/air (Koa) model: 1. 96E-009 Atmospheric Oxidation (25 deg C) [AopWin v1. 92]: Hydroxyl Radicals Reaction: OVERALL OH Rate Constant = 65. 5296 E-12

cm3/molecule-secHalf-Life = 0. 163 Days (12-hr day; 1. 5E6 OH/cm3)Half-Life = 1. 959 HrsOzone Reaction: No Ozone Reaction EstimationFraction sorbed to airborne particulates (phi): 8. 59E-010 (Junge, Mackay)Note: the sorbed fraction may be resistant to atmospheric oxidationSoil Adsorption Coefficient (PCKOCWIN v1. 66): Koc : 13. 4Log Koc: 1. 127 Aqueous Base/Acid-Catalyzed Hydrolysis (25 deg C) [HYDROWIN v1. 67]: Rate constants can NOT be estimated for this structure! Bioaccumulation Estimates from Log Kow (BCFWIN v2. 17): Log BCF from regression-based method = 0. 500 (BCF = 3. 162)log Kow used: -0. 38 (expkow database)Volatilization from Water: Henry LC: 1. 77E-005 atm-m3/mole (Henry experimental database)Half-Life from Model River: 22. 89 hoursHalf-Life from Model Lake : 306. 1 hours (12. 75 days)Removal In Wastewater Treatment: Total removal: 2. 81 percentTotal biodegradation: 0. 09 percentTotal sludge adsorption: 1. 74 percentTotal to Air: 0. 98 percent(using 10000 hr Bio P, A, S)Level III Fugacity Model: Mass Amount Half-Life Emissions(percent) (hr) (kg/hr)Air 0. 712 3. 78 1000 Water 48. 9 360 1000 Soil 50. 3 720 1000 Sediment 0. 0898 3. 24e+003 0 Persistence Time: 304 hr

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