2-aminopropane c3h9n structure

ASSIGN BUSTER

Contents

- Retention Index (Normal Alkane):

Molecular Formula	C_3H_9N
Average mass	59. 110 Da
Density	0. 7±0. 1 g/cm ^{3}
Boiling Point	30. 9±8. 0 °C at 760 mmHg
Flash Point	-32. 2±0. 0 °C
Molar Refractivity	19. 4±0. 3 cm ^{3}
Polarizability	7. 7±0. 5 10 $^{-24}$ cm ^{3}
Surface Tension	22. 0±3. 0 dyne/cm
Molar Volume	82. 1±3. 0 cm ^{3}

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

- Experimental Physico-chemical Properties

Experimental Melting Point:

-101 °CAlfa Aesar

-95 °CJean-Claude Bradley Open Melting Point Dataset13115

-95. 13 °CJean-Claude Bradley Open Melting Point Dataset21295

-101 °CJean-Claude Bradley Open Melting Point Dataset7384

-101 °CAlfa AesarA15044

-101 °CLabNetworkLN00195372

-95. 1 °CFooDBFDB009650

Experimental Boiling Point:

33-34 °CAlfa Aesar

91 F (32. 7778 °C)NIOSHNT8400000

34 °CFood and Agriculture Organization of the United Nations2-Aminopropane

32 °CArkema[ARK12],[ARK13]

53 °CArkema[ARK12],[ARK13]

33-34 °CAlfa AesarA15044

33-34 °COakwood094589

33-34 °CLabNetworkLN00195372

- **Experimental Ionization Potent:**

  8. 72

  EvNIOSHNT8400000

- **Experimental Vapor Pressure:**

  460

  mmHgNIOSHNT8400000

- **Experimental Flash Point:**

  -32 °CAlfa Aesar

  -32 °CAlfa Aesar

  -32 °F (-35. 5556 °C)Alfa

  AesarA15044

  -18 °COakwood094589

  -20 °CLabNetworkLN00195372

- **Experimental Freezing Point:**

  -150 F (-101. 1111

  °C)NIOSHNT8400000

- **Experimental Gravity:**

  20 g/mLMerck Millipore1750, 4487

  0 g/mLArkema[ARK12],[ARK12],[ARK13],

  [ARK13]

  20 g/lMerck Millipore1750, 4487, 845053,

  807476

  0. 691 g/mLAlfa AesarA15044

  0. 688 g/mLOakwood094589

  0. 72 g/mLFluorochem094589

  0. 69 g/lFluorochem094589

- **Experimental Refraction Index:**

  1. 3746Alfa AesarA15044

  1. 367-1. 373Food and Agriculture Organization of the United

  Nations2-Aminopropane

- **Experimental Solubility:**

  MiscibleNIOSHNT84000

00

- Miscellaneous

Appearance:

Colorless liquid with an ammonia-like odor. [Note: A gas above 91F.]NIOSHNT8400000

Colourless to yellow liquid; Fishy ammonia aromaFood and Agriculture Organization of the United Nations2-Aminopropane

Safety:

12-36/37/38Alfa AesarA15044

16-26-29Alfa AesarA15044

3Alfa AesarA15044

DangerAlfa AesarA15044

DANGER: FLAMMABLE, irritates skin and eyesAlfa AesarA15044

DANGER: FLAMMABLE, POISON, CORROSIVE, irritantAlfa AesarA15044

H224-H315-H319-H335Alfa AesarA15044

P210-P261-P303+P361+P353-P305+P351+P338-P405-P501aAlfa AesarA15044

- **First-Aid:**

  Eye: Irrigate immediately Skin: Water flush immediately Breathing: Resp

  support Swallow: Medical attention immediatelyNIOSHNT8400000

- **Exposure Routes:**

  inhalation, skin absorption, ingestion, skin and/or eye

  contactNIOSHNT8400000

- **Symptoms:**

  Irritation eyes, skin, nose, throat; pulmonary edema; visual disturbance;

  burns; dermatitisNIOSHNT8400000

- **Target Organs:**

  Eyes, skin, respiratory

  systemNIOSHNT8400000

- **Incompatibility:**

  Strong acids, strong oxidizers, aldehydes, ketones,

  epoxidesNIOSHNT8400000

- **Personal Protection:**

  Skin: Prevent skin contact Eyes: Prevent eye contact Wash skin: When

  contaminated Remove: When wet (flammable) Change: No recommenda

  Provide: Eyewash, Quick drenchNIOSHNT8400000

- **Exposure Limits:**

  NIOSH REL : See Appendix D OSHA PEL ?: TWA 5 ppm (12 mg/m

  3)NIOSHNT8400000

- Gas Chromatography

- **Retention Index (Kovats):**

  498 (estimated with error: 83)NIST Spectramainlib_341956, replib_1545(

  replib_229257

  469 (Program type: Isothermal; Col... (show more)umn class: Standard n

  Column length: 1 m; Column type: Packed; Start T: 130 C; CAS no: 7531(

  phase: OV-101; Carrier gas: Ar; Substrate: Chromosorb W HP; Data type:

  RI; Authors: Osmialowski, K.; Halkiewicz, J.; Radecki, A.; Kaliszan, R., Qua

  chemical parameters in correlation analysis of gas-liquid chromatographi

  retention indices of amines, J. Chromatogr., 346, 1985, 53-60.)NIST Spec

  468 (Program type: Isothermal; Col... (show more)umn class: Standard n

  Column length: 3 m; Column type: Packed; Start T: 180 C; CAS no: 7531(

  phase: SE-30; Carrier gas: N2; Substrate: Chromosorb W AW; Data type:

  RI; Authors: Oszczapowicz, J.; Osek, J.; Dolecka, E., Retention indices of

  dimethylformamidines, dimethylacetamidines and tetramethylguanidines

  non-polar column, J. Chromatogr., 315, 1984, 95-100.)NIST Spectranist ri

  477 (Program type: Isothermal; Col... (show more)umn class: Semi-stand

  polar; Column length: 2. 7 m; Column type: Packed; Start T: 100 C; CAS n

  75310; Active phase: Apiezon L; Carrier gas: N2 or He; Substrate: Chrom

  AW; Data type: Kovats RI; Authors: Zhuravleva, I. L.; Kapustin, Yu. P.; Gol

P. B., Retention indices of some isoaliphatic and heterocyclic nitrogenous
Zh. Anal. Khim., 31, 1976, 1378-1380.)NIST Spectranist ri

710 (Program type: Isothermal; Col… (show more)umn class: Standard p
Column length: 3 m; Column type: Packed; Start T: 179 C; CAS no: 7531(
phase: PEG-2000; Carrier gas: He; Substrate: Celite 545 (44-60 mesh); D
Kovats RI; Authors: Anderson, A.; Jurel, S.; Shymanska, M.; Golender, L.,
liquid chromatography of some aliphatic and heterocyclic mono- and
pollyfunctional amines. VII. Retention indices of amines in some polar an
unpolar stationary phases, Latv. PSR Zinat. Akad. Vestis Kim. Ser., , 1973
63.)NIST Spectranist ri

725 (Program type: Isothermal; Col… (show more)umn class: Standard p
Column length: 3 m; Column type: Packed; Start T: 152 C; CAS no: 7531(
phase: PEG-2000; Carrier gas: He; Substrate: Celite 545 (44-60 mesh); D
Kovats RI; Authors: Anderson, A.; Jurel, S.; Shymanska, M.; Golender, L.,
liquid chromatography of some aliphatic and heterocyclic mono- and
pollyfunctional amines. VII. Retention indices of amines in some polar an
unpolar stationary phases, Latv. PSR Zinat. Akad. Vestis Kim. Ser., , 1973
63.)NIST Spectranist ri

740 (Program type: Isothermal; Col… (show more)umn class: Standard p
Column length: 3 m; Column type: Packed; Start T: 150 C; CAS no: 7531(
phase: PEG-2000; Carrier gas: He; Substrate: Celite 545 (44-60 mesh); D
Kovats RI; Authors: Anderson, A.; Jurel, S.; Shymanska, M.; Golender, L.,
liquid chromatography of some aliphatic and heterocyclic mono- and
pollyfunctional amines. VII. Retention indices of amines in some polar an

unpolar stationary phases, Latv. PSR Zinat. Akad. Vestis Kim. Ser., , 1973
Program type: Isothermal; Col... (show more)umn class: Standard polar;
length: 3 m; Column type: Packed; Start T: 180 C; CAS no: 75310; Active
PEG-2000; Carrier gas: He; Substrate: Celite 545 (44-60 mesh); Data typ
RI; Authors: Anderson, A.; Jurel, S.; Shymanska, M.; Golender, L., Gas-liqu
chromatography of some aliphatic and heterocyclic mono- and pollyfunct
amines. VII. Retention indices of amines in some polar and unpolar static
phases, Latv. PSR Zinat. Akad. Vestis Kim. Ser., , 1973, 51-63.)NIST Spec

743 (Program type: Isothermal; Col... (show more)umn class: Standard p
Column length: 3 m; Column type: Packed; Start T: 120 C; CAS no: 75310
phase: PEG-2000; Carrier gas: He; Substrate: Celite 545 (44-60 mesh); D
Kovats RI; Authors: Anderson, A.; Jurel, S.; Shymanska, M.; Golender, L.,
liquid chromatography of some aliphatic and heterocyclic mono- and
pollyfunctional amines. VII. Retention indices of amines in some polar an
unpolar stationary phases, Latv. PSR Zinat. Akad. Vestis Kim. Ser., , 1973
63.)NIST Spectranist ri

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

  465 (Program type: Ramp; Column cl... (show more)ass: Standard non-po
  Column diameter: 0. 20 mm; Column length: 25 m; Column type: Capilla
  rate: 6 K/min; Start T: 50 C; End T: 250 C; CAS no: 75310; Active phase:
  Carrier gas: N2/He; Phase thickness: 0. 10 um; Data type: Normal alkane
  Authors: Zenkevich, I. G., Experimentally measured retention indices., 20
  Program type: Ramp; Column cl... (show more)ass: Standard non-polar;
  type: Capillary; CAS no: 75310; Active phase: Polydimethyl siloxanes; Da

Normal alkane RI; Authors: Zenkevich, I. G.; Chupalov, A. A., New Possibi
Chromato Mass Pectrometric Identification of Organic Compounds Using
Increments of Gas Chromatographic Retention Indices of Molecular Struc
Fragments, Zh. Org. Khim. (Rus.), 32(5), 1996, 656-666, In original 656-6
Spectranist ri

469 (Program type: Isothermal; Col… (show more)umn class: Standard n
Column type: Capillary; Start T: 130 C; CAS no: 75310; Active phase: OV-
Data type: Normal alkane RI; Authors: Qi, Y.; Yang, J.; Xu, L., correlation a
of the structures and gas liquid chromatographic retention indices of am
Chin. J. Anal. Chem., 28(2), 2000, 223-227.)NIST Spectranist ri

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

Density:	0. 7±0. 1 g/cm ^{3}
Boiling Point:	30. 9±8. 0 °C at 760 mmHg
Vapour Pressure:	607. 7±0. 1 mmHg at 25°C
Enthalpy of Vaporization:	27. 8±0. 0 kJ/mol
Flash Point:	-32. 2±0. 0 °C
Index of Refraction:	1. 389
Molar Refractivity:	19. 4±0. 3 cm ^{3}
#H bond acceptors:	1

#H bond donors:	2
#Freely Rotating Bonds:	0
#Rule of 5 Violations:	0
ACD/LogP:	0. 21
ACD/LogD (pH 5. 5):	-2. 76
ACD/BCF (pH 5. 5):	1. 00
ACD/KOC (pH 5. 5):	1. 00
ACD/LogD (pH 7. 4):	-2. 54
ACD/BCF (pH 7. 4):	1. 00
ACD/KOC (pH 7. 4):	1. 00
Polar Surface Area:	26 Å ^{2}
Polarizability:	7. 7±0. 5 10 $^{-24}$ cm ^{3}
Surface Tension:	22. 0±3. 0 dyne/cm
Molar Volume:	82. 1±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. 27Log Kow (Exper. database match) = 0. 26Exper. Ref: Hansch, C et al. (1995)Boiling Pt, Melting Pt, Vapor Pressure Estimations (MPBPWIN v1. 42): Boiling Pt (deg C): 47. 27 (Adapted Stein & Brown method)Melting Pt (deg C): -83. 69 (Mean or Weighted MP)VP(mm Hg, 25 deg C): 592 (Mean VP of Antoine & Grain methods)MP (exp database): -95. 1 deg CBP (exp database): 31. 7 deg CVP (exp database): 5. 80E+02 mm Hg at 25 deg CWater Solubility Estimate from Log Kow (WSKOW v1. 41): Water Solubility at 25 deg C (mg/L): 8. 381e+005log Kow used: 0. 26 (expkow database)no-melting pt equation usedWater Sol (Exper. database match) = 1e+006 mg/L (25 deg C)Exper. Ref: DORIGAN, J ET AL. (1976) @2NDWater Sol Estimate from Fragments: Wat Sol (v1. 01 est) = 6. 5379e+005 mg/LWat Sol (Exper. database match) = 1000000. 00Exper. Ref: DORIGAN, J ET AL. (1976) @2NDECOSAR Class Program (ECOSAR v0. 99h): Class(es) found: Aliphatic AminesHenrys Law Constant (25 deg C) [HENRYWIN v3. 10]: Bond Method : 1. 34E-005 atm-m3/moleGroup Method: IncompleteExper Database: 4. 51E-05 atm-m3/moleHenrys LC [VP/WSol estimate using EPI values]: 5. 494E-005 atm-m3/moleLog Octanol-Air Partition Coefficient (25 deg C) [KOAWIN v1. 10]: Log Kow used: 0. 26 (exp database)Log Kaw used: -2. 734 (exp database)Log Koa (KOAWIN v1. 10 estimate): 2. 994Log Koa (experimental database): NoneProbability of Rapid Biodegradation (BIOWIN v4. 10): Biowin1 (Linear Model) : 0. 8732Biowin2 (Non-Linear Model) : 0. 9637Expert Survey Biodegradation Results: Biowin3 (Ultimate Survey Model): 3. 0930 (weeks)Biowin4 (Primary Survey Model) : 3. 8057 (days)MITI Biodegradation Probability: Biowin5 (MITI Linear Model) : 0. 5197Biowin6 (MITI Non-Linear Model): 0. 6163Anaerobic Biodegradation Probability: Biowin7 (Anaerobic Linear Model): 0. 6884Ready 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): 7. 73E+004 Pa (580 mm Hg)Log Koa (Koawin est): 2. 994Kp (particle/gas partition coef. (m3/ug)): Mackay model : 3. 88E-011 Octanol/air (Koa) model: 2. 42E-010 Fraction sorbed to airborne particulates (phi): Junge-Pankow model : 1. 4E-009 Mackay model : 3. 1E-009 Octanol/air (Koa) model: 1. 94E-008 Atmospheric Oxidation (25 deg C) [AopWin v1. 92]: Hydroxyl Radicals Reaction: OVERALL OH Rate Constant = 39. 3766 E-12 cm3/molecule-secHalf-Life = 0. 272 Days (12-hr day; 1. 5E6 OH/cm3)Half-Life = 3. 260 HrsOzone Reaction: No Ozone Reaction EstimationFraction sorbed to airborne particulates (phi): 2. 25E-009 (Junge, Mackay)Note: the sorbed fraction may be resistant to atmospheric oxidationSoil Adsorption Coefficient (PCKOCWIN v1. 66): Koc : 26. 32Log Koc: 1. 420 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. 26 (expkow database)Volatilization from Water: Henry LC: 4. 51E-005 atm-m3/mole (Henry experimental database)Half-Life from Model River: 10. 77 hoursHalf-Life from Model Lake : 181. 9 hours (7. 579 days)Removal In Wastewater Treatment: Total removal: 4. 19 percentTotal biodegradation: 0. 09 percentTotal sludge adsorption: 1. 73 percentTotal to Air: 2. 38 percent(using 10000 hr Bio P, A, S)Level III Fugacity Model: Mass Amount Half-Life Emissions(percent) (hr) (kg/hr)Air 1. 52 6. 52 1000 Water 48. 9 360 1000 Soil 49. 5 720 1000 Sediment 0. 091 3. 24e+003 0 Persistence Time: 272 hr

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- 1-Click Docking

- 1-Click Scaffold Hop