1,1-dimethylhydrazine c2h8n2 structure

ASSIGN BUSTER

Contents

- Retention Index (Normal Alkane):

Molecular Formula	$C_2H_8N_2$
Average mass	60. 098 Da
Density	0. 8±0. 1 g/cm ^{3}
Boiling Point	63. 9±9. 0 °C at 760 mmHg
Flash Point	1. 1±0. 0 °C
Molar Refractivity	18. 6±0. 3 cm ^{3}
Polarizability	7. 4±0. 5 10^{-24} cm ^{3}
Surface Tension	27. 8±3. 0 dyne/cm
Molar Volume	72. 5±3. 0 cm ^{3}

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

- Experimental Physico-chemical Properties

  - **Experimental Melting Point:**

    -58 °CJean-Claude Bradley Open Melting Point Dataset21394

    -57 °CBiosynthQ-200052

  - **Experimental Boiling Point:**

    147 F (63. 8889 °C)NIOSHMV2450000

    61 °CBiosynthQ-200052

    60-62 °CSynQuest3139-1-02

  - **Experimental Ionization Potent:**

    8. 05 EvNIOSHMV2450000

  - **Experimental Vapor Pressure:**

    103 mmHgNIOSHMV2450000

  - **Experimental Flash Point:**

    5 F (-15 °C)NIOSHMV2450000

-10 °CBiosynthQ-200052

-10 °CSynQuest3139-1-02

- **Experimental Freezing Point:**

  -72 F (-57. 7778

  °C)NIOSHMV2450000

- **Experimental Gravity:**

  20 g/mLMerck Millipore2287

  20 g/lMerck Millipore2287,

  810408

  0. 79 g/mLBiosynthQ-200052

  0. 79 g/mLSynQuest3139-1-

  02

- **Experimental Solubility:**

  MiscibleNIOSHMV24500

  00

- Miscellaneous

  - **Appearance:**

    Colorless liquid with an ammonia- or fish-like odor.

NIOSHMV2450000

- **Safety:**

  DangerBiosynthQ-200052

  GHS02; GHS05; GHS06; GHS08; GHS09BiosynthQ-200052

  H225; H301; H314; H331; H350; H411BiosynthQ-200052

  Highly Flammable/Toxic/Corrosive/Carcinogenic/Keep ColdSynQuest3139-1-02

  Highly Flammable/Toxic/Corrosive/Keep ColdSynQuest3139-1-02

  P201; P210; P261; P273; P280; P301+P310BiosynthQ-200052

- **First-Aid:**

  Eye: Irrigate immediately Skin: Water flush immediately Breathing: Resp support Swallow: Medical attention immediatelyNIOSHMV2450000

- **Exposure Routes:**

  inhalation, skin absorption, ingestion, skin and/or eye contactNIOSHMV2450000

- **Symptoms:**

  Irritation eyes, skin; choking, chest pain, dyspnea (breathing difficulty); drowsiness; nausea; anoxia; convulsions; liver injury; [potential occupati

carcinogen]NIOSHMV2450000

- **Target Organs:**

  central nervous system, liver, gastrointestinal tract, blood, respiratory sy

  eyes, skin Cancer Site [in animals: tumors of the lungs, liver, blood vesse

  intestines]NIOSHMV2450000

- **Incompatibility:**

  Oxidizers, halogens, metallic mercury, fuming nitric acid, hydrogen perox

  [Note: May ignite SPONTANEOUSLY in contact with oxidizers.]NIOSHMV24

- **Personal Protection:**

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

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

  Provide: Eyewash, Quick drenchNIOSHMV2450000

- **Exposure Limits:**

  NIOSH REL : Ca C 0. 06 ppm (0. 15 mg/m 3) [2-hr] See Appendix A OSHA

  TWA 0. 5 ppm (1 mg/m 3) [skin]NIOSHMV2450000

- Gas Chromatography

  - **Retention Index (Kovats):**

    512 (estimated with error: 83)NIST Spectramainlib_229632,

    replib_161136, replib_64423

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

  527 (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: 57147; Active phase: C

  Carrier gas: N2/He; Phase thickness: 0. 10 um; Data type: Normal alkane

  Authors: Zenkevich, I. G., Experimentally measured retention indices.,

  2005.)NIST Spectranist ri

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

Density:	0. 8±0. 1 g/cm ^{3}
Boiling Point:	63. 9±9. 0 °C at 760 mmHg
Vapour Pressure:	167. 9±0. 1 mmHg at 25°C
Enthalpy of Vaporization:	30. 6±3. 0 kJ/mol
Flash Point:	1. 1±0. 0 °C
Index of Refraction:	1. 426
Molar Refractivity:	18. 6±0. 3 cm ^{3}
#H bond acceptors:	2
#H bond donors:	2
#Freely Rotating Bonds:	0

#Rule of 5 Violations:	0
ACD/LogP:	-1. 28
ACD/LogD (pH 5. 5):	-3. 28
ACD/BCF (pH 5. 5):	1. 00
ACD/KOC (pH 5. 5):	1. 00
ACD/LogD (pH 7. 4):	-1. 59
ACD/BCF (pH 7. 4):	1. 00
ACD/KOC (pH 7. 4):	1. 29
Polar Surface Area:	29 Å ^{2}
Polarizability:	7. 4±0. 5 10 $^{-24}$ cm ^{3}
Surface Tension:	27. 8±3. 0 dyne/cm
Molar Volume:	72. 5±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) = -1. 19Boiling Pt, Melting Pt, Vapor Pressure Estimations (MPBPWIN v1. 42): Boiling Pt (deg C): 62. 03 (Adapted Stein & Brown method)Melting Pt (deg C): -61. 29 (Mean or Weighted MP)VP(mm Hg, 25 deg C): 168 (Mean VP of Antoine & Grain methods)MP (exp database): -58 deg CBP (exp database): 63. 9 deg CVP

(exp database): 1. 63E+02 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: -1. 19 (estimated)no-melting pt equation usedWater Sol (Exper. database match) = 1e+006 mg/L (deg C)Exper. Ref: MERCK INDEX (1996)Water Sol Estimate from Fragments: Wat Sol (v1. 01 est) = 1e+006 mg/LWat Sol (Exper. database match) = 1000000. 00Exper. Ref: MERCK INDEX (1996)ECOSAR Class Program (ECOSAR v0. 99h): Class(es) found: HydrazinesHenrys Law Constant (25 deg C) [HENRYWIN v3. 10]: Bond Method : 6. 95E-008 atm-m3/moleGroup Method: IncompleteHenrys LC [VP/WSol estimate using EPI values]: 1. 329E-005 atm-m3/moleLog Octanol-Air Partition Coefficient (25 deg C) [KOAWIN v1. 10]: Log Kow used: -1. 19 (KowWin est)Log Kaw used: -5. 546 (HenryWin est)Log Koa (KOAWIN v1. 10 estimate): 4. 356Log Koa (experimental database): NoneProbability of Rapid Biodegradation (BIOWIN v4. 10): Biowin1 (Linear Model) : 0. 7189Biowin2 (Non-Linear Model) : 0. 8962Expert Survey Biodegradation Results: Biowin3 (Ultimate Survey Model): 3. 0664 (weeks)Biowin4 (Primary Survey Model) : 3. 7610 (days)MITI Biodegradation Probability: Biowin5 (MITI Linear Model) : 0. 1612Biowin6 (MITI Non-Linear Model): 0. 0000Anaerobic Biodegradation Probability: Biowin7 (Anaerobic Linear Model): 0. 6769Ready Biodegradability Prediction: NOHydrocarbon Biodegradation (BioHCwin v1. 01): Structure incompatible with current estimation method! Sorption to aerosols (25 Dec C)[AEROWIN v1. 00]: Vapor pressure (liquid/subcooled): 2. 17E+004 Pa (163 mm Hg)Log Koa (Koawin est): 4. 356Kp (particle/gas partition coef. (m3/ug)): Mackay model : 1. 38E-010 Octanol/air (Koa) model: 5. 57E-009 Fraction sorbed to airborne particulates (phi): Junge-Pankow model : 4. 99E-009 Mackay model : 1. 1E-008 Octanol/air (Koa) model: 4. 46E-007 Atmospheric Oxidation (25 deg C) [AopWin v1. 92]: Hydroxyl Radicals Reaction: OVERALL OH Rate Constant = 2. 5296 E-12 cm3/molecule-secHalf-Life = 4. 228 Days (12-hr day; 1. 5E6 OH/cm3)Half-Life = 50. 740 HrsOzone Reaction: No Ozone Reaction EstimationFraction sorbed to airborne particulates (phi): 8. 01E-009 (Junge, Mackay)Note: the sorbed fraction may be resistant to atmospheric oxidationSoil Adsorption Coefficient (PCKOCWIN v1. 66): Koc : 19. 78Log Koc: 1. 296 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: -1. 19 (estimated)Volatilization from Water: Henry LC: 6. 95E-008 atm-m3/mole (estimated by Bond SAR Method)Half-Life from Model River: 6532 hours (272. 1 days)Half-Life from Model Lake : 7. 132E+004 hours (2972 days)Removal In Wastewater Treatment: Total removal: 1. 85 percentTotal biodegradation: 0. 09 percentTotal sludge adsorption: 1. 75 percentTotal to Air: 0. 00 percent(using 10000 hr Bio P, A, S)Level III Fugacity Model: Mass Amount Half-Life Emissions(percent) (hr) (kg/hr)Air 0. 0396 0. 274 1000 Water 47. 9 360 1000 Soil 51. 9 720 1000 Sediment 0. 0877 3. 24e+003 0 Persistence Time: 344 hr

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