Acetylene c2h2 structure

Contents

Molecular Formula	C_2H_2
Average mass	26. 037 Da
Density	0. 6±0. 1 g/cm ^{3}
Boiling Point	-84. 0±9. 0 °C at 760 mmHg
Flash Point	-118. 7±12. 9 °C
Molar Refractivity	9. 0±0. 3 cm ^{3}
Polarizability	3. 6±0. 5 10 $^{-24}$ cm ^{3}
Surface Tension	16. 0±3. 0 dyne/cm
Molar Volume	45. 8±3. 0 cm ^{3}

- **Experimental Melting Point:**

  -80. 8 °COxford University Chemical Safety Data (No longer updated)

  -80. 8 °CJean-Claude Bradley Open Melting Point Dataset15571

  -80. 7 °CJean-Claude Bradley Open Melting Point Dataset21323

- **Experimental Boiling Point:**

  -84 °C (Sublimes)Oxford University Chemical Safety Data (No longer updated)

- **Experimental Ionization Potent:**

  11. 4 EvNIOSHAO9600000

- **Experimental Vapor Pressure:**

  44. 2 atm (33592 mmHg)NIOSHAO9600000

- **Experimental LogP:**

  0. 37Egon Willighagenhttp://dx. doi. org/10. 1021/ci050282s

- **Experimental Freezing Point:**

  -119 F (-83. 8889 °C)

  (Sublimes)NIOSHAO9600000

- **Experimental Solubility:**

  2%NIOSHAO960000

  0

- Miscellaneous

  - **Appearance:**

    Colorless gas with a faint, ethereal odor. [Note: Commercial grade has a

    like odor. Shipped under pressure dissolved in acetone.]NIOSHAO960000

    Colourless gas with garlic-like ordourOxford University Chemical Safety D

    longer updated)

  - **Stability:**

    Stable. Extremely flammable. Readily forms explosivemixtures with air. E

    small amounts of acetylene/airmixtures (for example a balloon the size o

    grapefruit) can produce damaging explosions if the mix is closeto stoichi

    Therefore acetylene/air explosions, if carried outas part of a chemistry sh

    classroom demonstration, should be approached with extreme caution. O

    University Chemical Safety Data (No longer updated)

  - **Toxicity:**

    http://ptcl. chem. ox. ac. uk/MSDS/AB/abamectin. htmlOxford University

Safety Data (No longer updated)

- **Safety:**

  Safety glasses. Good ventilation. Use ear protection ifdoing an acetylene
  explosion as a demonstration and take appropriate precautionsto prever
  to your audience! 2000 mg kg-1Oxford University Chemical Safety Data
  longer updated)

- **First-Aid:**

  Eye: Frostbite Skin: Frostbite Breathing: Fresh
  airNIOSHAO9600000

- **Exposure Routes:**

  inhalation, skin and/or eye contact
  (liquid)NIOSHAO9600000

- **Symptoms:**

  Headache, dizziness; asphyxia; liquid:
  frostbiteNIOSHAO9600000

- **Target Organs:**

  central nervous system, respiratory
  systemNIOSHAO9600000

- **Incompatibility:**

  Zinc; oxygen & other oxidizing agents such as halogens [Note: Forms ex

acetylide compounds with copper, mercury, silver & brasses (containing than 66% copper).]NIOSHAO9600000

- **Personal Protection:**

  Skin: Frostbite Eyes: Frostbite Wash skin: No recommendation Remove: wet (flammable) Change: No recommendation Provide: Frostbite washNIOSHAO9600000

- **Exposure Limits:**

  NIOSH REL : C 2500 ppm (2662 mg/m 3) OSHA PEL : noneNIOSHAO9600000

- Gas Chromatography

  - **Retention Index (Kovats):**

    198 (estimated with error: 39)NIST Spectramainlib_18810, replib_18811,

    195 (Program type: Complex; Column... (show more)class: Standard non- Column diameter: 0. 32 mm; Column length: 60 m; Column type: Capilla Description: -40 C for 12 min; -40 – 125 C at 3 deg. min; 125-185 C at 6 d 185 – 220 C at 20 deg/min; hold 220 C for 2 min; CAS no: 74862; Active p DB-1; Carrier gas: He; Phase thickness: 1. 0 um; Data type: Kovats RI; Au Hoekman, S. K., Improved gas chromatography procedure for speciated hydrocarbon measurements of vehicle emissions, J. Chromatogr., 639, 19 253.)NIST Spectranist ri

    155 (Program type: Isothermal; Col... (show more)umn class: Semi-stand polar; Column diameter: 0. 25 mm; Column length: 50 ft; Column type: P

Start T: 27 C; CAS no: 74862; Active phase: Squalane; Carrier gas: He; Su
Chromosorb P; Data type: Kovats RI; Authors: Hively, R. A.; Hinton, R. E.,
Variation of the retention index with temperature on squalane substrates
Chromatogr., 6, 1968, 203-217.)NIST Spectranist ri

156 (Program type: Isothermal; Col... (show more)umn class: Semi-stand
polar; Column diameter: 0. 25 mm; Column length: 50 ft; Column type: P
Start T: 67 C; CAS no: 74862; Active phase: Squalane; Carrier gas: He; Su
Chromosorb P; Data type: Kovats RI; Authors: Hively, R. A.; Hinton, R. E.,
Variation of the retention index with temperature on squalane substrates
Chromatogr., 6, 1968, 203-217., Program type: Isothermal; Col... (show
more)umn class: Semi-standard non-polar; Column diameter: 0. 25 mm;
length: 50 ft; Column type: Packed; Start T: 86 C; CAS no: 74862; Active
Squalane; Carrier gas: He; Substrate: Chromosorb P; Data type: Kovats R
Authors: Hively, R. A.; Hinton, R. E., Variation of the retention index with
temperature on squalane substrates, J. Gas Chromatogr., 6, 1968, 203-2
Spectranist ri

157 (Program type: Isothermal; Col... (show more)umn class: Semi-stand
polar; Column diameter: 0. 25 mm; Column length: 50 ft; Column type: P
Start T: 49 C; CAS no: 74862; Active phase: Squalane; Carrier gas: He; Su
Chromosorb P; Data type: Kovats RI; Authors: Hively, R. A.; Hinton, R. E.,
Variation of the retention index with temperature on squalane substrates
Chromatogr., 6, 1968, 203-217.)NIST Spectranist ri

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

156 (Program type: Ramp; Column cl... (show more)ass: Standard non-po

Column type: Capillary; CAS no: 74862; Active phase: Methyl Silicone; Da
Normal alkane RI; Authors: Chen, Y.; Feng, C., QSPR study on gas
chromatography retention index of some organic pollutants, Comput. Ap
Chem. (China), 24(10), 2007, 1404-1408.)NIST Spectranist ri

176 (Program type: Ramp; Column cl… (show more)ass: Semi-standard n
polar; Column length: 2 m; Column type: Packed; Heat rate: 5 K/min; Sta
C; End T: 220 C; End time: 0 min; Start time: 0 min; CAS no: 74862; Activ
Porapack Q; Carrier gas: Nitrogen; Data type: Normal alkane RI; Authors:
Zenkevich, I. G.; Konukhova, S. V., Gas Chromatographic Identification of
Ecologically Safe Freones, Vestn. of St. Petersburg Univ. (Rus.), , 1992, 6
original 66-70., Program type: Ramp; Column cl… (show more)ass: Stand
polar; Column diameter: 0. 20 mm; Column length: 25 m; Column type: C
Heat rate: 6 K/min; Start T: 50 C; End T: 250 C; CAS no: 74862; Active ph
101; Carrier gas: N2/He; Phase thickness: 0. 10 um; Data type: Normal a
Authors: Zenkevich, I. G., Experimentally measured retention indices.,
2005.)NIST Spectranist ri

155 (Program type: Ramp; Column cl… (show more)ass: Standard non-po
Column type: Capillary; CAS no: 74862; Active phase: Methyl Silicone; Da
Normal alkane RI; Authors: Du, X., Quantitative structure-property relatio
study on analysis of retention index of organic compound in gas
chromatography, Chemical World (Chinese), 42(8), 2001, 403-406.)NIST
Spectranist ri

165 (Program type: Complex; Column… (show more)class: Standard non-
Column diameter: 0. 53 mm; Column length: 60 m; Column type: Capilla

Description: 40C(6min)=> 5C/min=> 80C=> 10C/min=> 200C; CAS no:
Active phase: SPB-1; Carrier gas: He; Phase thickness: 5 um; Data type: I
alkane RI; Authors: Flanagan, R. J.; Streete, P. J.; Ramsey, J. D., Volatile S
Abuse, UNODC Technical Series, No 5, United Nations, Office on Drugs ar
Crime, Vienna International Centre, PO Box 500, A-1400 Vienna, Austria,
56.)NIST Spectranist ri

182 (Program type: Ramp; Column cl... (show more)ass: Semi-standard r
polar; Column type: Capillary; CAS no: 74862; Active phase: Porapack Q;
type: Normal alkane RI; Authors: Zenkevich, I. G.; Rodin, A. A., Gas
chromatographic identification of some volatile toxic fluorine containing
compounds by precalculated retention indices, J. Ecol. Chem. (Rus.), 13(1
22-28.)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:	-84. 0±9. 0 °C at 760 mmHg
Vapour Pressure:	69690. 6±0. 1 mmHg at 25°C
Enthalpy of Vaporization:	21. 1±0. 8 kJ/mol
Flash Point:	-118. 7±12. 9 °C
Index of Refraction:	1. 316

Molar Refractivity:	9. 0±0. 3 cm^{3}
#H bond acceptors:	0
#H bond donors:	0
#Freely Rotating Bonds:	0
#Rule of 5 Violations:	0
ACD/LogP:	0. 37
ACD/LogD (pH 5. 5):	0. 43
ACD/BCF (pH 5. 5):	1. 24
ACD/KOC (pH 5. 5):	40. 62
ACD/LogD (pH 7. 4):	0. 43
ACD/BCF (pH 7. 4):	1. 24
ACD/KOC (pH 7. 4):	40. 62
Polar Surface Area:	0 $Å^{2}$
Polarizability:	3. 6±0. 5 10^{-24} cm^{3}
Surface Tension:	16. 0±3. 0 dyne/cm
Molar Volume:	45. 8±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. 50Log Kow (Exper. database match) = 0. 37Exper. Ref: Hansch, C et al. (1995)Boiling Pt, Melting Pt, Vapor Pressure Estimations (MPBPWIN v1. 42): Boiling Pt (deg C): -36. 63 (Adapted Stein & Brown method)Melting Pt (deg C): -154. 04 (Mean or Weighted MP)VP(mm Hg, 25 deg C): 1. 81E+004 (Mean VP of Antoine & Grain methods)MP (exp database): -80. 7 deg CBP (exp database): -84. 7 deg CVP (exp database): 4. 04E+04 mm Hg at 25 deg CWater Solubility Estimate from Log Kow (WSKOW v1. 41): Water Solubility at 25 deg C (mg/L): 1. 476e+004log Kow used: 0. 37 (expkow database)no-melting pt equation usedWater Sol (Exper. database match) = 1200 mg/L (20 deg C)Exper. Ref: YALKOWSKY, SH & DANNENFELSER, RM (1992)Water Sol Estimate from Fragments: Wat Sol (v1. 01 est) = 12559 mg/LWat Sol (Exper. database match) = 1200. 00Exper. Ref: YALKOWSKY, SH & DANNENFELSER, RM (1992)ECOSAR Class Program (ECOSAR v0. 99h): Class(es) found: Neutral OrganicsHenrys Law Constant (25 deg C) [HENRYWIN v3. 10]: Bond Method : 2. 40E-002 atm-m3/moleGroup Method: 2. 45E-002 atm-m3/moleExper Database: 2. 17E-02 atm-m3/moleHenrys LC [VP/WSol estimate using EPI values]: 1. 764E-003 atm-m3/moleLog Octanol-Air Partition Coefficient (25 deg C) [KOAWIN v1. 10]: Log Kow used: 0. 37 (exp database)Log Kaw used: -0. 052 (exp database)Log Koa (KOAWIN v1. 10 estimate): 0. 422Log Koa (experimental database): NoneProbability of Rapid Biodegradation (BIOWIN v4. 10): Biowin1 (Linear Model) : 0. 7351Biowin2 (Non-Linear Model) : 0. 9333Expert Survey Biodegradation Results: Biowin3 (Ultimate Survey Model): 3. 1416 (weeks)Biowin4 (Primary Survey Model) : 3. 8102 (days)MITI Biodegradation Probability: Biowin5 (MITI Linear Model) : 0. 6347Biowin6 (MITI Non-Linear Model): 0. 8550Anaerobic Biodegradation Probability: Biowin7 (Anaerobic Linear Model): 0. 8361Ready Biodegradability Prediction: YESHydrocarbon Biodegradation (BioHCwin v1. 01): LOG BioHC Half-Life (days) : 0. 4898BioHC Half-Life (days) : 3. 0886Sorption to aerosols (25 Dec C) [AEROWIN v1. 00]: Vapor pressure (liquid/subcooled): 5. 39E+006 Pa (4. 04E+004 mm Hg)Log Koa (Koawin est): 0. 422Kp (particle/gas partition coef. (m3/ug)): Mackay model : 5. 57E-013 Octanol/air (Koa) model: 6. 49E-013 Fraction sorbed to airborne particulates (phi): Junge-Pankow model : 2. 01E-011 Mackay model : 4. 46E-011 Octanol/air (Koa) model: 5. 19E-011 Atmospheric Oxidation (25 deg C) [AopWin v1. 92]: Hydroxyl Radicals Reaction: OVERALL OH Rate Constant = 0. 8150 E-12 cm3/molecule-secHalf-Life = 13. 124 Days (12-hr day; 1. 5E6 OH/cm3)Ozone Reaction: OVERALL Ozone Rate Constant = 0. 003000 E-17 cm3/molecule-secHalf-Life = 382. 000 Days (at 7E11 mol/cm3)Fraction sorbed to airborne particulates (phi): 3. 23E-011 (Junge, Mackay)Note: the sorbed fraction may be resistant to atmospheric oxidationSoil Adsorption Coefficient (PCKOCWIN v1. 66): Koc : 14. 3Log Koc: 1. 155 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. 37 (expkow database)Volatilization from Water: Henry LC: 0. 0217 atm-m3/mole (Henry experimental database)Half-Life from Model River: 0. 5345 hours (32. 07 min)Half-Life from Model Lake : 48. 62 hours (2. 026 days)Removal In Wastewater Treatment: Total removal: 89. 42 percentTotal biodegradation: 0. 03 percentTotal sludge adsorption: 0. 41 percentTotal to Air: 88. 98 percent(using 10000 hr Bio P, A, S)Level III Fugacity Model: Mass Amount Half-Life Emissions(percent) (hr) (kg/hr)Air 50. 9 298 1000 Water 47. 6 360 1000 Soil 1. 44 720 1000 Sediment 0. 089 3. 24e+003 0 Persistence Time: 130 hr

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