

# [Acetylene c2h2 structure](https://assignbuster.com/acetylene-c2h2-structure/)

Contents

* Retention Index (Normal Alkane):

|  |  |
| --- | --- |
| Molecular Formula | C 2 H 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 data
* Predicted – ACD/Labs
* Predicted – EPISuite
* Predicted – ChemAxon
* Experimental Physico-chemical Properties

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| -80. 8 °COxford University Chemical Safety Data (No longer updated) |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

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| -84 °C (Sublimes)Oxford University Chemical Safety Data (No longer updated) |

## Experimental Ionization Potent:

|  |
| --- |
| 11. 4 EvNIOSHAO9600000 |

## Experimental Vapor Pressure:

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| --- |
| 44. 2 atm (33592 mmHg)NIOSHAO9600000 |

## Experimental LogP:

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

## Experimental Freezing Point:

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| --- |
| -119 F (-83. 8889 °C)(Sublimes)NIOSHAO9600000 |

## Experimental Solubility:

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| --- |
| 2%NIOSHAO9600000 |

* Miscellaneous

## Appearance:

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| Colorless gas with a faint, ethereal odor. [Note: Commercial grade has a garlic-like odor. Shipped under pressure dissolved in acetone.]NIOSHAO9600000 |
| Colourless gas with garlic-like ordourOxford University Chemical Safety Data (No longer updated) |

## Stability:

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| --- |
| Stable. Extremely flammable. Readily forms explosivemixtures with air. Even small amounts of acetylene/airmixtures (for example a balloon the size of a grapefruit) can produce damaging explosions if the mix is closeto stoichiometric. Therefore acetylene/air explosions, if carried outas part of a chemistry show or a classroom demonstration, should be approached with extreme caution. Oxford University Chemical Safety Data (No longer updated) |

## Toxicity:

|  |
| --- |
| http://ptcl. chem. ox. ac. uk/MSDS/AB/abamectin. htmlOxford University Chemical Safety Data (No longer updated) |

## Safety:

|  |
| --- |
| Safety glasses. Good ventilation. Use ear protection ifdoing an acetylene/air explosion as a demonstration and take appropriate precautionsto prevent harm to your audience! 2000 mg kg-1Oxford University Chemical Safety Data (No longer updated) |

## First-Aid:

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| --- |
| Eye: Frostbite Skin: Frostbite Breathing: Fresh airNIOSHAO9600000 |

## Exposure Routes:

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

## Symptoms:

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| Headache, dizziness; asphyxia; liquid: frostbiteNIOSHAO9600000 |

## Target Organs:

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| central nervous system, respiratory systemNIOSHAO9600000 |

## Incompatibility:

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| Zinc; oxygen & other oxidizing agents such as halogens [Note: Forms explosive acetylide compounds with copper, mercury, silver & brasses (containing more than 66% copper).]NIOSHAO9600000 |

## Personal Protection:

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

## Exposure Limits:

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

* Gas Chromatography

## Retention Index (Kovats):

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| --- |
| 198 (estimated with error: 39)NIST Spectramainlib\_18810, replib\_18811, replib\_8 |
| 195 (Program type: Complex; Column… (show more)class: Standard non-polar; Column diameter: 0. 32 mm; Column length: 60 m; Column type: Capillary; Description: -40 C for 12 min; -40 – 125 C at 3 deg. min; 125-185 C at 6 deg/min; 185 – 220 C at 20 deg/min; hold 220 C for 2 min; CAS no: 74862; Active phase: DB-1; Carrier gas: He; Phase thickness: 1. 0 um; Data type: Kovats RI; Authors: Hoekman, S. K., Improved gas chromatography procedure for speciated hydrocarbon measurements of vehicle emissions, J. Chromatogr., 639, 1993, 239-253.)NIST Spectranist ri |
| 155 (Program type: Isothermal; Col… (show more)umn class: Semi-standard non-polar; Column diameter: 0. 25 mm; Column length: 50 ft; Column type: Packed; Start T: 27 C; CAS no: 74862; Active phase: Squalane; Carrier gas: He; Substrate: Chromosorb P; Data type: Kovats RI; Authors: Hively, R. A.; Hinton, R. E., Variation of the retention index with temperature on squalane substrates, J. Gas Chromatogr., 6, 1968, 203-217.)NIST Spectranist ri |
| 156 (Program type: Isothermal; Col… (show more)umn class: Semi-standard non-polar; Column diameter: 0. 25 mm; Column length: 50 ft; Column type: Packed; Start T: 67 C; CAS no: 74862; Active phase: Squalane; Carrier gas: He; Substrate: Chromosorb P; Data type: Kovats RI; Authors: Hively, R. A.; Hinton, R. E., Variation of the retention index with temperature on squalane substrates, J. Gas Chromatogr., 6, 1968, 203-217., Program type: Isothermal; Col… (show more)umn class: Semi-standard non-polar; Column diameter: 0. 25 mm; Column length: 50 ft; Column type: Packed; Start T: 86 C; CAS no: 74862; Active phase: Squalane; Carrier gas: He; Substrate: Chromosorb P; Data type: Kovats RI; Authors: Hively, R. A.; Hinton, R. E., Variation of the retention index with temperature on squalane substrates, J. Gas Chromatogr., 6, 1968, 203-217.)NIST Spectranist ri |
| 157 (Program type: Isothermal; Col… (show more)umn class: Semi-standard non-polar; Column diameter: 0. 25 mm; Column length: 50 ft; Column type: Packed; Start T: 49 C; CAS no: 74862; Active phase: Squalane; Carrier gas: He; Substrate: Chromosorb P; Data type: Kovats RI; Authors: Hively, R. A.; Hinton, R. E., Variation of the retention index with temperature on squalane substrates, J. Gas Chromatogr., 6, 1968, 203-217.)NIST Spectranist ri |

## Retention Index (Normal Alkane):

|  |
| --- |
| 156 (Program type: Ramp; Column cl… (show more)ass: Standard non-polar; Column type: Capillary; CAS no: 74862; 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 |
| 176 (Program type: Ramp; Column cl… (show more)ass: Semi-standard non-polar; Column length: 2 m; Column type: Packed; Heat rate: 5 K/min; Start T: 50 C; End T: 220 C; End time: 0 min; Start time: 0 min; CAS no: 74862; Active phase: 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, 66-70, In original 66-70., 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: 74862; 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 |
| 155 (Program type: Ramp; Column cl… (show more)ass: Standard non-polar; Column type: Capillary; CAS no: 74862; Active phase: Methyl Silicone; Data type: Normal alkane RI; Authors: Du, X., Quantitative structure-property relationship 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-polar; Column diameter: 0. 53 mm; Column length: 60 m; Column type: Capillary; Description: 40C(6min)=> 5C/min=> 80C=> 10C/min=> 200C; CAS no: 74862; Active phase: SPB-1; Carrier gas: He; Phase thickness: 5 um; Data type: Normal alkane RI; Authors: Flanagan, R. J.; Streete, P. J.; Ramsey, J. D., Volatile Substance Abuse, UNODC Technical Series, No 5, United Nations, Office on Drugs and Crime, Vienna International Centre, PO Box 500, A-1400 Vienna, Austria, 1997, 56.)NIST Spectranist ri |
| 182 (Program type: Ramp; Column cl… (show more)ass: Semi-standard non-polar; Column type: Capillary; CAS no: 74862; Active phase: Porapack Q; Data 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), 2004, 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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