

# [Hydrogen sulfide h2s structure](https://assignbuster.com/hydrogen-sulfide-h2s-structure/)

Contents

* Retention Index (Normal Alkane):

|  |  |
| --- | --- |
| Molecular Formula  | H 2 S  |
| Average mass  | 34. 081 Da  |
| Density  |  |
| Boiling Point  | -60. 7±9. 0 °C at 760 mmHg  |
| Flash Point  |  |
| Molar Refractivity  |  |
| Polarizability  |  |
| Surface Tension  |  |
| Molar Volume  |  |

* Experimental data
* Predicted – ACD/Labs
* Predicted – EPISuite
* Predicted – ChemAxon
* Experimental Physico-chemical Properties

## Experimental Melting Point:

|  |
| --- |
| 116 °COxford University Chemical Safety Data (No longer updated)More details  |
| -85 °COxford University Chemical Safety Data (No longer updated)More details  |
| -85. 49 °CJean-Claude Bradley Open Melting Point Dataset22451  |
| 112 °CJean-Claude Bradley Open Melting Point Dataset25712  |

## Experimental Boiling Point:

|  |
| --- |
| -77 F (-60. 5556 °C)NIOSHMX1225000  |
| 445 °COxford University Chemical Safety Data (No longer updated)More details  |
| -60 °COxford University Chemical Safety Data (No longer updated)More details  |

## Experimental Ionization Potent:

|  |
| --- |
| 10. 46 EvNIOSHMX1225000  |

## Experimental Vapor Pressure:

|  |
| --- |
| 17. 6 atm (13376 mmHg)NIOSHMX1225000  |

## Experimental Flash Point:

|  |
| --- |
| 188 °COxford University Chemical Safety Data (No longer updated)More details  |
| -82 °COxford University Chemical Safety Data (No longer updated)More details  |

## Experimental Freezing Point:

|  |
| --- |
| -122 F (-85. 5556 °C)NIOSHMX1225000  |

## Experimental Solubility:

|  |
| --- |
| 0. 4%NIOSHMX1225000  |

* Miscellaneous

## Appearance:

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| Colorless gas with a strong odor of rotten eggs. [Note: Sense of smell becomes rapidly fatigued & can NOT be relied upon to warn of the continuous presence of H2S. Shipped as a liquefied compressed gas.]NIOSHMX1225000  |
| colourless gas with strong odour of rotten eggs (odour threshold ca 0. 2 ppt)Oxford University Chemical Safety Data (No longer updated)More details  |
| yellow powder or fused solid, or amber to yellow crystalsOxford University Chemical Safety Data (No longer updated)More details  |

## Stability:

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| --- |
| Stable. Highly flammable. May form explosive mixture with air. Note wide explosive limits. Incompatible with strong oxidizing agents, many metals. May react violently with metal oxides, copper, fluorine, sodium, ethanal. Oxford University Chemical Safety Data (No longer updated)More details  |
| Stable. Dust may form a flammable or explosive mixture with air. Incompatible with strong oxidizing agents, most common metals, hydrogen, chlorine, fluorine. Oxford University Chemical Safety Data (No longer updated)More details  |

## Safety:

|  |
| --- |
| FAbblis ChemicalsAB1002328  |
| GHS07BiosynthQ-201771  |
| H315; H319; H335BiosynthQ-201771  |
| P261; P280; P302+P352; P304+P340; P305+P351+P338; P312BiosynthQ-201771  |
| Safety glasses, rubber gloves, good ventilation. Remove all sourcesof ignition from the working area. Oxford University Chemical Safety Data (No longer updated)More details  |
| Safety glasses. Oxford University Chemical Safety Data (No longer updated)More details  |
| WarningBiosynthQ-201771  |

## First-Aid:

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| --- |
| Eye: Frostbite Skin: Frostbite Breathing: Respiratory supportNIOSHMX1225000  |

## Exposure Routes:

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| --- |
| inhalation, skin and/or eye contactNIOSHMX1225000  |

## Symptoms:

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| Irritation eyes, respiratory system; apnea, coma, convulsions; conjunctivitis, eye pain, lacrimation (discharge of tears), photophobia (abnormal visual intolerance to light), corneal vesiculation; dizziness, headache, lassitude (weakness, exhaustion), irritability, insomnia; gastrointestinal disturbance; liquid: frostbiteNIOSHMX1225000  |

## Target Organs:

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| --- |
| Eyes, respiratory system, central nervous systemNIOSHMX1225000  |

## Incompatibility:

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| Strong oxidizers, strong nitric acid, metalsNIOSHMX1225000  |

## Personal Protection:

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| --- |
| Skin: Frostbite Eyes: Frostbite Wash skin: No recommendation Remove: When wet (flammable) Change: No recommendation Provide: Frostbite washNIOSHMX1225000  |

## Exposure Limits:

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| --- |
| NIOSH REL : C 10 ppm (15 mg/m 3 ) [10-minute] OSHA PEL ?: C 20 ppm 50 ppm [10-minute maximum peak]NIOSHMX1225000  |

* Gas Chromatography

## Retention Index (Normal Alkane):

|  |
| --- |
| 438 (Program type: Ramp; Column cl… (show more)ass: Standard non-polar; Column diameter: 0. 20 mm; Column length: 50 m; Column type: Capillary; CAS no: 7783064; Active phase: PONA; Phase thickness: 0. 50 um; Data type: Normal alkane RI; Authors: Yang, Y.-T.; Wang, Z.; Han. J.-H.; Tian, H.-P.; Yang, H.-Y., Determination of sulfur compounds in gasoline fraction of microreactor products by gas chromatography – Atomic emission detector, Petrochemical Technology (Shiyou Huagong), 32(11), 2003, 995-998., Program type: Ramp; Column cl… (show more)ass: Standard non-polar; Column diameter: 0. 20 mm; Column length: 50 m; Column type: Capillary; Heat rate: 2 K/min; Start T: 30 C; End T: 150 C; CAS no: 7783064; Active phase: PONA; Phase thickness: 0. 50 um; Data type: Normal alkane RI; Authors: Yang, Y.-T.; Wang, Z.; Han. J.-H.; Tian, H.-P.; Yang, H.-Y., Determination of sulfur compounds in gasoline fraction of microreactor products by gas chromatography – Atomic emission detector, Petrochemical Technology (Shiyou Huagong), 32(11), 2003, 995-998.)NIST Spectranist ri  |
| 480 (Program type: Ramp; Column cl… (show more)ass: Standard polar; Column diameter: 0. 25 mm; Column length: 60 m; Column type: Capillary; Heat rate: 3 K/min; Start T: 70 C; End T: 220 C; End time: 40 min; CAS no: 7783064; Active phase: TC-Wax; Carrier gas: N2; Phase thickness: 0. 25 um; Data type: Normal alkane RI; Authors: Ishizaki, S.; Tachihara, T.; Tamura, H.; Yanai, T.; Kitahara, T., Evaluation of odour-active compounds in roasted shrimp (Sergia lucens Hansen) by aroma extract dilution analysis, Flavour Fragr. J., 20, 2005, 562-566., Program type: Ramp; Column cl… (show more)ass: Standard polar; Column type: Capillary; CAS no: 7783064; Active phase: TC-Wax; Data type: Normal alkane RI; Authors: Tachihara, T.; Ishizaki, S.; Ishikawa, M.; Kitahara, T., Studies on the volatile compounds of roasted spotted shrimp, Chemistry & Biodiversity, 1, 2004, 2024-2033.)NIST Spectranist ri  |

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

|  |  |
| --- | --- |
| Density:  |  |
| Boiling Point:  | -60. 7±9. 0 °C at 760 mmHg  |
| Vapour Pressure:  | 12581. 3±0. 1 mmHg at 25°C  |
| Enthalpy of Vaporization:  | 18. 7±0. 0 kJ/mol  |
| Flash Point:  |  |
| Index of Refraction:  |  |
| Molar Refractivity:  |  |
| #H bond acceptors:  | 0  |
| #H bond donors:  | 0  |
| #Freely Rotating Bonds:  | 0  |
| #Rule of 5 Violations:  |  |

|  |  |
| --- | --- |
| ACD/LogP:  |  |
| ACD/LogD (pH 5. 5):  |  |
| ACD/BCF (pH 5. 5):  |  |
| ACD/KOC (pH 5. 5):  |  |
| ACD/LogD (pH 7. 4):  |  |
| ACD/BCF (pH 7. 4):  |  |
| ACD/KOC (pH 7. 4):  |  |
| Polar Surface Area:  | 0 Å 2  |
| Polarizability:  |  |
| Surface Tension:  |  |
| Molar Volume:  |  |

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. 23Log Kow (Exper. database match) = -1. 38Exper. Ref: Hansch, C et al. (1995)Boiling Pt, Melting Pt, Vapor Pressure Estimations (MPBPWIN v1. 42): Boiling Pt (deg C): 473. 12 (Adapted Stein & Brown method)Melting Pt (deg C): 173. 17 (Mean or Weighted MP)VP(mm Hg, 25 deg C): 35. 2 (Mean VP of Antoine & Grain methods)MP (exp database): 3. 81 deg CBP (exp database): 101. 42 deg CVP (exp database): 2. 06E+01 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. 38 (expkow database)no-melting pt equation usedWater Sol (Exper. database match) = 4. 82e+005 mg/L (24 deg C)Exper. Ref: DEAN, JA (1985)Water Sol (Exper. database match) = 3740 mg/L (21 deg C)Exper. Ref: VANABLE, CS & FUWA, T (1922)Water Sol Estimate from Fragments: Wat Sol (v1. 01 est) = 60488 mg/LWat Sol (Exper. database match) = 482000. 00Exper. Ref: DEAN, JA (1985)Wat Sol (Exper. database match) = 3740. 00Exper. Ref: VANABLE, CS & FUWA, T (1922)ECOSAR Class Program (ECOSAR v0. 99h): Class(es) found: Neutral OrganicsHenrys Law Constant (25 deg C) [HENRYWIN v3. 10]: Bond Method : 8. 69E-003 atm-m3/moleGroup Method: IncompleteHenrys LC [VP/WSol estimate using EPI values]: 1. 578E-006 atm-m3/moleLog Octanol-Air Partition Coefficient (25 deg C) [KOAWIN v1. 10]: Log Kow used: -1. 38 (exp database)Log Kaw used: -0. 449 (HenryWin est)Log Koa (KOAWIN v1. 10 estimate): -0. 931Log Koa (experimental database): NoneProbability of Rapid Biodegradation (BIOWIN v4. 10): Biowin1 (Linear Model) : 0. 7313Biowin2 (Non-Linear Model) : 0. 9259Expert Survey Biodegradation Results: Biowin3 (Ultimate Survey Model): 3. 1239 (weeks )Biowin4 (Primary Survey Model) : 3. 7986 (days )MITI Biodegradation Probability: Biowin5 (MITI Linear Model) : 0. 6108Biowin6 (MITI Non-Linear Model): 0. 8237Anaerobic Biodegradation Probability: Biowin7 (Anaerobic Linear Model): 0. 8361Ready 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. 75E+003 Pa (20. 6 mm Hg)Log Koa (Koawin est ): -0. 931Kp (particle/gas partition coef. (m3/ug)): Mackay model : 1. 09E-009 Octanol/air (Koa) model: 2. 88E-014 Fraction sorbed to airborne particulates (phi): Junge-Pankow model : 3. 95E-008 Mackay model : 8. 74E-008 Octanol/air (Koa) model: 2. 3E-012 Atmospheric Oxidation (25 deg C) [AopWin v1. 92]: Hydroxyl Radicals Reaction: OVERALL OH Rate Constant = 0. 0000 E-12 cm3/molecule-secHalf-Life = -------Ozone Reaction: No Ozone Reaction EstimationFraction sorbed to airborne particulates (phi): 6. 34E-008 (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: -1. 38 (expkow database)Volatilization from Water: Henry LC: 0. 00869 atm-m3/mole (estimated by Bond SAR Method)Half-Life from Model River: 0. 635 hours (38. 10 min)Half-Life from Model Lake : 55. 88 hours (2. 328 days)Removal In Wastewater Treatment: Total removal: 77. 40 percentTotal biodegradation: 0. 03 percentTotal sludge adsorption: 0. 59 percentTotal to Air: 76. 77 percent(using 10000 hr Bio P, A, S)Level III Fugacity Model: Mass Amount Half-Life Emissions(percent) (hr) (kg/hr)Air 55 1e+005 1000 Water 42. 6 360 1000 Soil 2. 33 720 1000 Sediment 0. 0779 3. 24e+003 0 Persistence Time: 148 hr

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