Hydrogen sulfide h2s structure

Contents

Molecular Formula	H_2S
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 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)NIOSHMX1225

  000

- **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:**

    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.]NIOSHMX122500

    0

    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ca 0. 2 ppt)Oxford University Chemical Safety Data (No longer updated)More details

yellow powder or fused solid, or amber to yellow crystalsOxford University Chemical Safety Data (No longer updated)More details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:**

  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Oxford University Chemical Safety Data (No longer updated)More details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Oxford University Chemical Safety Data (No longer updated)More details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:**

  Eye: Frostbite Skin:

  Frostbite Breathing:

  Respiratory

  supportNIOSHMX1225

  000

- **Exposure Routes:**

  inhalation, skin and/or

  eye

  contactNIOSHMX1225

  000

- **Symptoms:**

  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:

frostbiteNIOSHMX1225

000

- **Target Organs:**

  Eyes, respiratory

  system, central

  nervous

  systemNIOSHMX12250

  00

- **Incompatibility:**

  Strong oxidizers,

  strong nitric acid,

  metalsNIOSHMX12250

  00

- **Personal Protection:**

  Skin: Frostbite Eyes:

  Frostbite Wash skin:

  No recommendation

  Remove: When wet

(flammable) Change:

No recommendation

Provide: Frostbite

washNIOSHMX122500

0

- **Exposure Limits:**

  NIOSH REL : C 10 ppm

  (15 mg/m 3) [10-

  minute] OSHA PEL ?: C

  20 ppm 50 ppm [10-

  minute maximum

  peak]NIOSHMX122500

  0

- 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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