Sulfathiazole c9h9n3o2s2 structure

Contents

- Retention Index (Kovats):

Molecular Formula	$C_9H_9N_3O_2S_2$
Average mass	255. 317 Da
Density	1. 6±0. 1 g/cm ^{3}
Boiling Point	479. 5±47. 0 °C at 760 mmHg
Flash Point	243. 8±29. 3 °C
Molar Refractivity	63. 5±0. 4 cm ^{3}
Polarizability	25. 2±0. 5 10^{-24} cm ^{3}
Surface Tension	83. 1±3. 0 dyne/cm
Molar Volume	163. 5±3. 0 cm ^{3}

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

- Predicted – ChemAxon
- Predicted – Mcule
- Experimental Physico-chemical Properties

Experimental Melting Point:

200 °CTCIS0272

200-203 °CAlfa Aesar

202 °COxford University Chemical Safety Data (No longer updated)More details

199-202 °CMerck Millipore3230, 821112

202. 5 °CJean-Claude Bradley Open Melting Point Dataset28555, 28556

200 °CJean-Claude Bradley Open Melting Point Dataset28555, 28556

202 °CJean-Claude

Bradley Open Melting

Point Dataset15438,

17204, 21528, 8442

200-203 °CAlfa

AesarA10727

80 °CBiosynthQ-

201766

196-198

°CLabNetworkLN00225

368

- **Experimental Flash Point:**

  102. 9 °CBiosynthQ-

  201766

- **Experimental Gravity:**

  102. 9 g/mLBiosynthQ-

  201766

- **Experimental Solubility:**

  10 mM in

  DMSOMedChem

ExpressHY-B0507

-2. 43Egon

Willighagenhttp://dx.

doi. org/10.

1021/ci050282s

DMSO 50 mg/mL;

Water <1

mg/mLMedChem

Expresshttp://www.

medchemexpress.

com/Sulfathiazole-

sodium. html, HY-

B0507

- Predicted Physico-chemical Properties

  - **Predicted Melting Point:**

    200 °CTCI

    200

    °CTCIS0272

- Miscellaneous

  - **Appearance:**

    white to cream

    powderOxford

University Chemical Safety Data (No longer updated)More details

- **Stability:**

  Stable. Incompatible with strong oxidizing agents. Oxford University Chemical Safety Data (No longer updated)More details

- **Toxicity:**

  IPR-MUS LD50 400 mg kg-1, SCU-MUS LD50 1450 mg kg-1, IVN-MUS LD50 990 mg kg-1Oxford University Chemical Safety Data (No longer updated)More details

- **Safety:**

  26-37Alfa AesarA10727

  36/37/38Alfa

AesarA10727

H315-H319-H335Alfa

AesarA10727

P261; P262BiosynthQ-

201766

P261-P280-

P305+P351+P338-

P304+P340-P405-

P501aAlfa

AesarA10727

Safety glasses,

adequate ventilation.

Oxford University

Chemical Safety Data

(No longer

updated)More details

WarningAlfa

AesarA10727

WARNING: Irreversible

damage risk, protect

skin/eyes/lungs. Alfa

AesarA10727

- **Target Organs:**

  Antibiotic; DHPS

  inhibitorTargetMolT074

  7

- **Compound Source:**

  syntheticMicrosource[0150

  0553]

- **Bio Activity:**

  AntibacterialMedChem

  ExpressHY-B0507

  Anti-infectionMedChem

  ExpressHY-B0507

  Anti-infection;

  MedChem ExpressHY-

  B0507

  Dihydropteroate

  synthetase;

  DHPSTargetMolT0747

  EnzymeTargetMolT074

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Sulfathiazole is an organosulfur compound that has been used as a short-acting sulfa drug.; Target: Antibacterial; Sulfathiazole (20 ? g/L) starts to be degraded between day 31 and day 38 in one of the two batch reactors containing different wastewater matrices. MedChem ExpressHY-B0507

Sulfonamide; Zerenex Molecular[ZBioX-0664]

- Gas Chromatography

- **Retention Index (Kovats):**

  2423 (estimated with error: 89)NIST Spectramainlib_231963, replib_290925,

replib_65076

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

Density:	1. 6±0. 1 g/cm ^{3}
Boiling Point:	479. 5±47. 0 °C at 760 mmHg
Vapour Pressure:	0. 0±1. 2 mmHg at 25°C
Enthalpy of Vaporization:	74. 4±3. 0 kJ/mol
Flash Point:	243. 8±29. 3 °C
Index of Refraction:	1. 704
Molar Refractivity:	63. 5±0. 4 cm ^{3}
#H bond acceptors:	5
#H bond donors:	3
#Freely Rotating Bonds:	3
#Rule of 5 Violations:	0
ACD/LogP:	0. 05
ACD/LogD (pH 5. 5):	0. 41
ACD/BCF (pH 5. 5):	1. 20

ACD/KOC (pH 5. 5):	39. 50
ACD/LogD (pH 7. 4):	0. 03
ACD/BCF (pH 7. 4):	1. 00
ACD/KOC (pH 7. 4):	16. 59
Polar Surface Area:	122 Å ^{2}
Polarizability:	25. 2±0. 5 10 $^{-24}$ cm ^{3}
Surface Tension:	83. 1±3. 0 dyne/cm
Molar Volume:	163. 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) = 0. 72Log Kow (Exper. database match) = 0. 05Exper. Ref: Hansch, C et al. (1995)Boiling Pt, Melting Pt, Vapor Pressure Estimations (MPBPWIN v1. 42): Boiling Pt (deg C): 428. 28 (Adapted Stein & Brown method)Melting Pt (deg C): 179. 10 (Mean or Weighted MP)VP(mm Hg, 25 deg C): 3. 24E-008 (Modified Grain method)MP (exp database): 189 deg CSubcooled liquid VP: 1. 69E-006 mm Hg (25 deg C, Mod-Grain method)Water Solubility Estimate from Log Kow (WSKOW v1. 41): Water Solubility at 25 deg C (mg/L): 2. 003e+004log Kow used: 0. 05 (expkow database)no-melting pt equation usedWater Sol (Exper. database match) = 373 mg/L (25 deg C)Exper. Ref: YALKOWSKY, SH & DANNENFELSER, RM (1992)Water Sol Estimate from Fragments: Wat Sol (v1. 01 est) = 671. 45 mg/LWat Sol (Exper. database match) = 373. 00Exper. Ref: YALKOWSKY, SH & DANNENFELSER, RM (1992)ECOSAR Class Program (ECOSAR v0. 99h): Class(es) found: Aromatic AminesHenrys Law Constant (25 deg C) [HENRYWIN v3. 10]: Bond Method : 5. 85E-014 atm-m3/moleGroup Method: IncompleteHenrys LC [VP/WSol estimate using EPI values]: 5. 434E-013 atm-m3/moleLog Octanol-Air Partition Coefficient (25 deg C) [KOAWIN v1. 10]: Log Kow used: 0. 05 (exp database)Log Kaw used: -11. 621 (HenryWin est)Log Koa (KOAWIN v1. 10 estimate): 11. 671Log Koa (experimental database): NoneProbability of Rapid Biodegradation (BIOWIN v4. 10): Biowin1

(Linear Model) : 0. 3922Biowin2 (Non-Linear Model) : 0. 0742Expert Survey Biodegradation Results: Biowin3 (Ultimate Survey Model): 2. 5000 (weeks-months)Biowin4 (Primary Survey Model) : 3. 3710 (days-weeks)MITI Biodegradation Probability: Biowin5 (MITI Linear Model) : -0. 1558Biowin6 (MITI Non-Linear Model): 0. 0047Anaerobic Biodegradation Probability: Biowin7 (Anaerobic Linear Model): -0. 0143Ready 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): 0. 000225 Pa (1. 69E-006 mm Hg)Log Koa (Koawin est): 11. 671Kp (particle/gas partition coef. (m3/ug)): Mackay model : 0. 0133 Octanol/air (Koa) model: 0. 115 Fraction sorbed to airborne particulates (phi): Junge-Pankow model : 0. 325 Mackay model : 0. 516 Octanol/air (Koa) model: 0. 902 Atmospheric Oxidation (25 deg C) [AopWin v1. 92]: Hydroxyl Radicals Reaction: OVERALL OH Rate Constant = 53. 6431 E-12 cm3/molecule-secHalf-Life = 0. 199 Days (12-hr day; 1. 5E6 OH/cm3)Half-Life = 2. 393 HrsOzone Reaction: No Ozone Reaction EstimationFraction sorbed to airborne particulates (phi): 0. 42 (Junge, Mackay)Note: the sorbed fraction may be resistant to atmospheric oxidationSoil Adsorption Coefficient (PCKOCWIN v1. 66): Koc : 945. 1Log Koc: 2. 975 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. 05 (expkow database)Volatilization from Water: Henry LC: 5. 85E-014 atm-m3/mole (estimated by Bond SAR Method)Half-Life from Model River: 1. 599E+010 hours (6. 663E+008 days)Half-Life from Model Lake : 1. 745E+011 hours (7. 269E+009 days)Removal In Wastewater Treatment: Total removal: 1. 85 percentTotal biodegradation: 0. 09 percentTotal sludge adsorption: 1. 76 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 1. 49e-006 4. 79 1000 Water 45. 7 900 1000 Soil 54. 2 1. 8e+003 1000 Sediment 0. 0887 8. 1e+003 0 Persistence Time: 983 hr

Click to predict properties on the Chemicalize site

- 1-Click Docking
- 1-Click Scaffold Hop