

# [Sulfathiazole c9h9n3o2s2 structure](https://assignbuster.com/sulfathiazole-c9h9n3o2s2-structure/)

Contents

* Retention Index (Kovats):

|  |  |
| --- | --- |
| Molecular Formula | C 9 H 9 N 3 O 2 S 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| 202 °COxford University Chemical Safety Data (No longer updated)More details |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 °CLabNetworkLN00225368 |

## 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| white to cream powderOxford University Chemical Safety Data (No longer updated)More details |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 Oxford University Chemical Safety Data (No longer updated)More details |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| IPR-MUS LD50 400 mg kg-1, SCU-MUS LD50 1450 mg kg-1, IVN-MUS LD50 990 mg kg-1Oxford University Chemical Safety Data (No longer updated)More details |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 Oxford University Chemical Safety Data (No longer updated)More details |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:

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| --- |
| Antibiotic; DHPS inhibitorTargetMolT0747 |

## Compound Source:

|  |
| --- |
| syntheticMicrosource[01500553] |

## Bio Activity:

|  |
| --- |
| AntibacterialMedChem ExpressHY-B0507 |
| Anti-infectionMedChem ExpressHY-B0507 |
| Anti-infection; MedChem ExpressHY-B0507 |
| Dihydropteroate synthetase; DHPSTargetMolT0747 |
| EnzymeTargetMolT0747 |
| 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

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* 1-Click Scaffold Hop