

Sulfadimethoxine

C12H14N4O4S
structure



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- Retention Index (Kovats):

Molecular

$C_{12}H_{14}N_4O_4S$

Formula

Average mass 310. 329 Da

Density 1. 4±0. 1 g/cm³

Boiling Point 548. 5±60. 0 °C at
760 mmHg

Flash Point 285. 5±32. 9 °C

Molar	
Refractivity	75. 9±0. 4 cm ³
Polarizability	30. 1±0. 5 10 ⁻²⁴ cm ³
Surface	
Tension	69. 5±3. 0 dyne/cm

Molar Volume 215. 3±3. 0 cm³

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

- **Experimental Melting Point:**

200 °CTCIS0359

201 °CLKT Labs[S8246]

203. 5 °CJean-Claude

Bradley Open Melting

Point Dataset21541,

28536, 28537, 28538

204. 5 °CJean-Claude

Bradley Open Melting

Point Dataset28536,

28537, 28538

200

°CLabNetworkLN00194

965

201-203

°CFooDBFDB010661

- **Experimental Solubility:**

10 mM in

DMSOMedChem

ExpressHY-B0337

10 mM in

H2OMedChem

ExpressHY-B0337

Soluble in dilute HCl,

and in aqueous

solutions of sodium

carbonate. LKT

Labs[S8246]

- Predicted Physico-chemical Properties

- **Predicted Melting Point:**

200 °CTCI

200

°CTCIS0359

- Miscellaneous

- **Safety:**

36/37/38-43LKT

Labs[S8246]

H315 H317 H319

H335LKT Labs[S8246]

NoneLKT Labs[S8246]

XiAbblis

ChemicalsAB1004582

XiLKT Labs[S8246]

- **Target Organs:**

AntibioticTargetMolT1

078

- **Drug Status:**

approvedBIONET-Key OrganicsKS-

5335

- **Compound Source:**

syntheticMicrosource[0150
1144]

- **Bio Activity:**

AntibacterialMedChem
ExpressHY-B0337

Anti-infectionMedChem
ExpressHY-B0337

Anti-infection;
MedChem ExpressHY-
B0337

Microbiology &
VirologyTargetMolT107
8

OthersTargetMolT1078

Sulfadimethoxine is a
sulfonamide antibiotic.
MedChem Express

Sulfadimethoxine is a

sulfonamide antibiotic.;

Target: Antibacterial;

Sulfadimethoxine is a sulfonamide antibiotic.

MedChem ExpressHY-B0337

Sulfadimethoxine is a sulfonamide antibiotic.;

Target:

AntibacterialSulfadimethoxine is a sulfonamide antibiotic.

Sulfadimethoxine is used to treat many infections including treatment of respiratory, urinary tract, enteric, and soft tissue infections. It is most frequently used in veterinary medicine, although it is approved in some countries for use in humans.

Sulfadimethoxine

inhibits bacterial
synthesis of folic acid
(pteroylglutamic acid)
from para-
aminobenzoic acid.

Sulfadimethoxine is
approved in Russia for
use in humans,
including children, and
has been successfully
used there for more
than 35 years. It is
widely available in
Russia as an over-the-
counter drug
manufactured by a
number of Russian
pharmaceutical
companies [1].

MedChem ExpressHY-
B0337

- Gas Chromatography

- **Retention Index (Kovats):**

2750 (estimated with
error: 89)NIST

Spectramainlib_236954

, replib_248693

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

Density:	1.4 ± 0.1 g/cm ³
Boiling Point:	548.5 ± 60.0 °C at 760 mmHg
Vapour Pressure:	0.0 ± 1.5 mmHg at 25°C
Enthalpy of Vaporization:	82.8 ± 3.0 kJ/mol
Flash Point:	285.5 ± 32.9 °C
Index of Refraction:	1.623
Molar Refractivity:	75.9 ± 0.4 cm ³
#H bond acceptors:	8
#H bond donors:	3
#Freely Rotating Bonds:	5
#Rule of 5 Violations:	0
ACD/LogP:	1.48
ACD/LogD (pH 5.5):	0.43

ACD/BCF (pH 5. 5):	1. 00
ACD/KOC (pH 5. 5):	13. 76
ACD/LogD (pH 7. 4):	-0. 49
ACD/BCF (pH 7. 4):	1. 00
ACD/KOC (pH 7. 4):	1. 66
Polar Surface Area:	125 Å ²
Polarizability:	30. 1±0. 5 10 ⁻²⁴ cm ³
Surface Tension:	69. 5±3. 0 dyne/cm
Molar Volume:	215. 3±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) = 1. 17Log Kow (Exper. database match) = 1. 63Exper. Ref: Hansch, C et al. (1995)Boiling Pt, Melting Pt, Vapor Pressure Estimations (MPBPWIN v1. 42): Boiling Pt (deg C): 475. 30 (Adapted Stein & Brown method)Melting Pt (deg C): 201. 06 (Mean or Weighted MP)VP(mm Hg, 25 deg C): 1. 49E-009 (Modified Grain method)MP (exp database): 203. 5 deg CSubcooled liquid VP: 1. 15E-007 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): 433. 1log Kow used: 1. 63 (expkow database)no-melting pt equation usedWater Sol (Exper. database match) = 343 mg/L (deg C)Exper. Ref: YALKOWSKY, SH & DANNENFELSER, RM (1992)Water Sol Estimate from Fragments: Wat Sol (v1. 01 est) = 3930. 6 mg/LWat Sol (Exper. database match) = 343. 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 : 1. 30E-014 atm-m³/moleGroup Method: IncompleteHenrys LC [VP/WSol estimate using EPI values]: 1. 405E-012 atm-m³/moleLog Octanol-Air Partition Coefficient (25 deg

<https://assignbuster.com/sulfadimethoxine-c12h14n4o4s-structure/>

C) [KOAWIN v1. 10]: Log Kow used: 1. 63 (exp database)Log Kaw used: -12. 275 (HenryWin est)Log Koa (KOAWIN v1. 10 estimate): 13. 905Log Koa (experimental database): NoneProbability of Rapid Biodegradation (BIOWIN v4. 10): Biowin1 (Linear Model) : 0. 6299Biowin2 (Non-Linear Model) : 0. 7670Expert Survey Biodegradation Results: Biowin3 (Ultimate Survey Model): 2. 2622 (weeks-months)Biowin4 (Primary Survey Model) : 3. 4459 (days-weeks)MITI Biodegradation Probability: Biowin5 (MITI Linear Model) : 0. 0636Biowin6 (MITI Non-Linear Model): 0. 0124Anaerobic Biodegradation Probability: Biowin7 (Anaerobic Linear Model): 0. 2780Ready 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): 1. 53E-005 Pa (1. 15E-007 mm Hg)Log Koa (Koawin est): 13. 905Kp (particle/gas partition coef. (m3/ug)): Mackay model : 0. 196 Octanol/air (Koa) model: 19. 7 Fraction sorbed to airborne particulates (phi): Junge-Pankow model : 0. 876 Mackay model : 0. 94 Octanol/air (Koa) model: 0. 999 Atmospheric Oxidation (25 deg C) [AopWin v1. 92]: Hydroxyl Radicals Reaction: OVERALL OH Rate Constant = 201. 6592 E-12 cm3/molecule-secHalf-Life = 0. 053 Days (12-hr day; 1. 5E6 OH/cm3)Half-Life = 0. 636 HrsOzone Reaction: No Ozone Reaction EstimationFraction sorbed to airborne particulates (phi): 0. 908 (Junge, Mackay)Note: the sorbed fraction may be resistant to atmospheric oxidationSoil Adsorption Coefficient (PCKOCWIN v1. 66): Koc : 95. 73Log Koc: 1. 981 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. 555 (BCF = 3. 59)log Kow used: 1. 63 (expkow database)Volatilization from Water: Henry LC: 1. 3E-014 atm-m3/mole (estimated by Bond SAR Method)Half-Life from Model River: 7. 934E+010 hours (3. 306E+009 days)Half-Life from Model Lake : 8. 655E+011 hours (3. 606E+010 days)Removal In Wastewater Treatment: Total removal: 2. 02 percentTotal biodegradation: 0. 09 percentTotal sludge adsorption: 1. 92 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. 71e-006 1. 27 1000 Water 30. 3 900 1000 Soil 69. 6 1. 8e+003 1000 Sediment 0. 0831 8. 1e+003 0 Persistence Time: 1. 24e+003 hr

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