Metronidazole c6h9n3o3 structure

Contents

- Retention Index (Linear):

Molecular Formula	$C_6H_9N_3O_3$
Average mass	171. 154 Da
Density	1. 5±0. 1 g/cm ^{3}
Boiling Point	405. 4±25. 0 °C at 760 mmHg
Flash Point	199. 0±23. 2 °C
Molar Refractivity	41. 0±0. 5 cm ^{3}
Polarizability	16. 2±0. 5 10 $^{-24}$ cm ^{3}
Surface Tension	60. 5±7. 0 dyne/cm
Molar Volume	117. 9±7. 0 cm ^{3}

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

- Experimental Physico-chemical Properties

Experimental Melting Point:

161 °CTCIM0924

158-162 °COxford

University Chemical Safety

Data (No longer

updated)More details

159-163 °CLKT

Labs[M1977]

159 °CJean-Claude

Bradley Open Melting

Point Dataset17317

160 °CJean-Claude

Bradley Open Melting

Point Dataset15095,

16645, 28269

159-161 °CAlfa

AesarH60258

159-161

°CSynQuest4H54-1-9A

160 °CBiosynthQ-201403

159-161

°CLabNetworkLN0019621

9

- **Experimental LogP:**

  -0. 013Vitas-MSTK177359,

  STK177359

- **Experimental Flash Point:**

  199 °CBiosynthQ-

  201403

- **Experimental Gravity:**

  199 g/mLBiosynthQ-

  201403

- **Experimental Solubility:**

  10 mM in H2OMedChem

  ExpressHY-B0318

  DMSO 35 mg/mL; Water

  <1 mg/mLMedChem

  ExpressHY-B0318

  Soluble in water, dilute

acids and ethanol. Slightly soluble in DMF. DMSO 34 mg/mL. LKT Labs[M1977]

- Predicted Physico-chemical Properties
  - **Predicted Melting Point:**

    161 °CTCI

    161

    °CTCIM0924

- Miscellaneous
  - **Appearance:**

    white to slightly yellow crystalline powderOxford University Chemical Safety Data (No longer updated)More details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 Oxford University Chemical Safety Data (No longer updated)More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:**

  ORL-RAT LD50 3000 mg kg-1, ORL-MUS LD50 3800 mg kg-1, SCU-MUS LD50 3640 mg kg-1Oxford University Chemical Safety Data (No longer updated)More details

- **Safety:**

  36/37-60Alfa AesarH60258

  40Alfa AesarH60258

  Carcinogenic/ MutagenicSynQuest4H54-1-9A

  H351Alfa AesarH60258

  P261; P262BiosynthQ-201403

  P281-P201-P202-P308+P313-P405-

P501aAlfa AesarH60258

Safety glasses, adequate

ventilation. Oxford

University Chemical Safety

Data (No longer

updated)More details

WarningAlfa AesarH60258

- **Target Organs:**

  Hydrogenase inhibitor;

  AntibioticTargetMolT1079

- **Drug Status:**

  approvedBIONET-Key OrganicsKS-

  5140

- **Compound Source:**

  syntheticMicrosource[0150

  0412]

- **Bio Activity:**

  . Zerenex

  Molecular[ZBioX-0563]

  AntibacterialMedChem

ExpressHY-B0318

Antibacterial

AntiparasiticMedChem

ExpressHY-B0318

Anti-infectionMedChem

ExpressHY-B0318

Anti-infection; MedChem

ExpressHY-B0318

Fe hydrogenase 1; NADPH

nitroreductase; 14-??

DemethylaseTargetMolT1

079

Metabolism; Microbiology

& VirologyTargetMolT1079

Metronidazole is a

nitroimidazole antibiotic

medication used

particularly for anaerobic

bacteria and protozoa.

MedChem Express

Metronidazole is a

nitroimidazole antibiotic

medication used particularly for anaerobic bacteria and protozoa.; Target: Antibacterial; Antiparasitic; Metronidazole is a nitroimidazole antibiotic medication used particularly for anaerobic bacteria and protozoa. MedChem ExpressHY-B0318

Metronidazole is a nitroimidazole antibiotic medication used particularly for anaerobic bacteria and protozoa.; Target: Antibacterial; AntiparasiticMetronidazole is a nitroimidazole antibiotic medication used particularly for anaerobic bacteria and protozoa. Metronidazole is an antibiotic, amebicide, and

antiprotozoal.[1] It is the drug of choice for first episodes of mild-to-moderate Clostridium difficile infection [2]. Metronidazole, taken up by diffusion, is selectively absorbed by anaerobic bacteria and sensitive protozoa. Once taken up by anaerobes, it is non-enzymatically reduced by reacting with reduced ferredoxin, which is generated by pyruvate oxido-reductase. Many of the reduced nitroso intermediates will form sulfinamides and thioether linkages with cysteine-bearing enzymes, thereby deactivating these critical enzymes. As many as 150 separate enzymes are affected. In addition or alternatively, the

metronidazole metabolites

are taken up into bacterial

DNA, and form

unstableMedChem

ExpressHY-B0318

- Gas Chromatography

  - **Retention Index (Kovats):**

    1518 (estimated with

    error: 89)NIST

    Spectramainlib_352184,

    replib_76026,

    replib_236890,

    replib_335158

    1618 (Program type:

    Isothermal; Col… (show

    more)umn class: Standard

    non-polar; Column length:

    2 m; Column type:

    Packed; Start T: 180 C;

    CAS no: 443481; Active

    phase: SE-30; Carrier gas:

    N2; Substrate: 1% se-30

    on Anachrom ABS(80-

    100mesh); Data type:

Kovats RI; Authors: Musumarra, G.; Scarlata, G.; Romano, G.; Cappello, G.; Clementi, S.; Giulietti, G., Qualitative organic analysis. Part 2. Identification of drugs by principal components analysis of standardized TLC data in four eluent systems and of retention indices on SE 30, J. Anal. Toxicol., 11, 1987, 154-163.)NIST Spectranist ri

- **Retention Index (Normal Alkane):**

  1643. 7 (Program type: Ramp; Column cl… (show more)ass: Standard non-polar; Column diameter: 0. 32 mm; Column length: 12 m; Column type: Capillary; Heat rate: 10 K/min; Start T: 40 C; End T: 290 C; Start time: 1 min; CAS no: 443481; Active phase: SE-

30; Carrier gas: He; Phase thickness: 0. 25 um; Data type: Normal alkane RI; Authors: Neill, G. P.; Davies, N. W.; McLean, S., Automated screening procedure using gas chromatography-mass spectrometry for identification of drugs after their extraction from biological samples, J. Chromatogr., 565, 1991, 207-224.)NIST Spectranist ri

1592 (Program type: Ramp; Column cl… (show more)ass: Standard non-polar; Column type: Other; CAS no: 443481; Active phase: Methyl Silicone; Data type: Normal alkane RI; Authors: Ardrey, R. E.; Moffat, A. C., Gas-liquid chromatographic retention

indices of 1318 substances of toxicological interest on SE-30 or OV-1 stationary phase, J. Chromatogr., 220, 1981, 195-252.)NIST Spectranist ri

- **Retention Index (Linear):**

  1590 (Program type: Ramp; Column cl… (show more)ass: Standard non-polar; Column length: 1. 8 m; Column type: Packed; Heat rate: 8 K/min; Start T: 130 C; End T: 290 C; End time: 8 min; Start time: 2 min; CAS no: 443481; Active phase: SE-30; Carrier gas: N2; Substrate: Chromosorb W; Data type: Linear RI; Authors: Perrigo, B. J.; Peel, H. W., The use of retention indices and temperature-programmed

gas chromatography in analytical toxicology, J. Chromatogr. Sci., 19, 1981, 219-226.)NIST Spectranist ri

1669. 6 (Program type: Complex; Column... (show more)class: Semi-standard non-polar; Column diameter: 0. 25 mm; Column length: 30 m; Column type: Capillary; Description: Multi-step temperature program; T(initial)= 60C; T(final)= 270C; CAS no: 443481; Active phase: VF-5MS; Carrier gas: He; Phase thickness: 0. 25 um; Data type: Linear RI; Authors: Tret’yakov, K. V., Retention Data. NIST Mass Spectrometry Data Center., 2008.)NIST

Spectranist ri

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

Density:	1. 5±0. 1 g/cm ^{3}
Boiling Point:	405. 4±25. 0 °C at 760 mmHg
Vapour Pressure:	0. 0±1. 0 mmHg at 25°C
Enthalpy of Vaporization:	69. 3±3. 0 kJ/mol
Flash Point:	199. 0±23. 2 °C
Index of Refraction:	1. 612
Molar Refractivity:	41. 0±0. 5 cm ^{3}
#H bond acceptors:	6
#H bond donors:	1
#Freely Rotating Bonds:	3
#Rule of 5 Violations:	0
ACD/LogP:	-0. 01
ACD/LogD (pH 5. 5):	0. 05
ACD/BCF (pH 5. 5):	1. 00

ACD/KOC (pH 5. 5):	25. 34
ACD/LogD (pH 7. 4):	0. 05
ACD/BCF (pH 7. 4):	1. 00
ACD/KOC (pH 7. 4):	25. 38
Polar Surface Area:	84 Å ^{2}
Polarizability:	16. 2±0. 5 10 $^{-24}$ cm ^{3}
Surface Tension:	60. 5±7. 0 dyne/cm
Molar Volume:	117. 9±7. 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. 00Log Kow (Exper. database match) = -0. 02Exper. Ref: Hansch, C et al. (1995)Boiling Pt, Melting Pt, Vapor Pressure Estimations (MPBPWIN v1. 42): Boiling Pt (deg C): 357. 30 (Adapted Stein & Brown method)Melting Pt (deg C): 127. 46 (Mean or Weighted MP)VP(mm Hg, 25 deg C): 1. 31E-007 (Modified Grain method)MP (exp database): 160. 5 deg CSubcooled liquid VP: 3. 22E-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. 573e+004log Kow used: -0. 02 (expkow database)no-melting pt equation usedWater Sol (Exper. database match) = 9500 mg/L (25 deg C)Exper. Ref: YALKOWSKY, SH & DANNENFELSER, RM (1992)Water Sol Estimate from Fragments: Wat Sol (v1. 01 est) = 3. 2779e+005 mg/LWat Sol (Exper. database match) = 9500. 00Exper. Ref: YALKOWSKY, SH & DANNENFELSER, RM (1992)ECOSAR Class Program (ECOSAR v0. 99h): Class(es) found: ImidazolesHenrys Law Constant (25 deg C) [HENRYWIN v3. 10]: Bond Method : 1. 69E-011 atm-m3/moleGroup Method: IncompleteHenrys LC [VP/WSol estimate using EPI values]: 1. 147E-012 atm-m3/moleLog Octanol-Air Partition Coefficient (25 deg C) [KOAWIN v1. 10]: Log Kow used: -0. 02 (exp database)Log Kaw used: -9. 161 (HenryWin est)Log Koa (KOAWIN v1. 10 estimate): 9. 141Log Koa (experimental database): NoneProbability of Rapid

Biodegradation (BIOWIN v4. 10): Biowin1 (Linear Model) : 0. 5744Biowin2 (Non-Linear Model) : 0. 4414Expert Survey Biodegradation Results: Biowin3 (Ultimate Survey Model): 2. 7365 (weeks-months)Biowin4 (Primary Survey Model) : 3. 5533 (days-weeks)MITI Biodegradation Probability: Biowin5 (MITI Linear Model) : 0. 3250Biowin6 (MITI Non-Linear Model): 0. 0739Anaerobic Biodegradation Probability: Biowin7 (Anaerobic Linear Model): 0. 3396Ready 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. 000429 Pa (3. 22E-006 mm Hg)Log Koa (Koawin est): 9. 141Kp (particle/gas partition coef. (m3/ug)): Mackay model : 0. 00699 Octanol/air (Koa) model: 0. 00034 Fraction sorbed to airborne particulates (phi): Junge-Pankow model : 0. 202 Mackay model : 0. 359 Octanol/air (Koa) model: 0. 0265 Atmospheric Oxidation (25 deg C) [AopWin v1. 92]: Hydroxyl Radicals Reaction: OVERALL OH Rate Constant = 9. 3017 E-12 cm3/molecule-secHalf-Life = 1. 150 Days (12-hr day; 1. 5E6 OH/cm3)Half-Life = 13. 799 HrsOzone Reaction: No Ozone Reaction EstimationFraction sorbed to airborne particulates (phi): 0. 28 (Junge, Mackay)Note: the sorbed fraction may be resistant to atmospheric oxidationSoil Adsorption Coefficient (PCKOCWIN v1. 66): Koc : 10Log Koc: 1. 000 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. 02 (expkow database)Volatilization from Water: Henry LC: 1. 69E-011 atm-m3/mole (estimated by Bond SAR Method)Half-Life from Model River: 4. 532E+007 hours (1. 888E+006 days)Half-Life from Model Lake : 4. 944E+008 hours (2. 06E+007 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 0. 000391 27. 6 1000 Water 45. 8 900 1000 Soil 54. 1 1. 8e+003 1000 Sediment 0. 0887 8. 1e+003 0 Persistence Time: 981 hr

Click to predict properties on the Chemicalize site

- 1-Click Docking
- 1-Click Scaffold Hop