

# [Metronidazole c6h9n3o3 structure](https://assignbuster.com/metronidazole-c6h9n3o3-structure/)

Contents

* Retention Index (Linear):

|  |  |
| --- | --- |
| Molecular Formula | C 6 H 9 N 3 O 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| 158-162 °COxford University Chemical Safety Data (No longer updated)More details |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 °CLabNetworkLN00196219 |

## 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| white to slightly yellow crystalline powderOxford University Chemical Safety Data (No longer updated)More details |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 Oxford University Chemical Safety Data (No longer updated)More details |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ORL-RAT LD50 3000 mg kg-1, ORL-MUS LD50 3800 mg kg-1, SCU-MUS LD50 3640 mg kg-1Oxford University Chemical Safety Data (No longer updated)More details |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 Oxford University Chemical Safety Data (No longer updated)More details |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[01500412] |

## 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-?? DemethylaseTargetMolT1079 |
| 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