

# [Trimebutine c22h29no5 structure](https://assignbuster.com/trimebutine-c22h29no5-structure/)

\n[toc title="Table of Contents"]\n

\n \t

1. [Experimental Melting Point:](#experimental-melting-point) \n \t
2. [Experimental LogP:](#experimental-logp) \n \t
3. [Experimental Solubility:](#experimental-solubility) \n \t
4. [Safety:](#safety) \n \t
5. [Target Organs:](#target-organs) \n \t
6. [Bio Activity:](#bio-activity) \n \t
7. [Retention Index (Kovats):](#retention-index-kovats) \n

\n[/toc]\n \n

Contents

* Retention Index (Kovats):

|  |  |
| --- | --- |
| Molecular Formula  | C 22 H 29 NO 5  |
| Average mass  | 387. 469 Da  |
| Density  | 1. 1±0. 1 g/cm 3  |
| Boiling Point  | 457. 9±34. 0 °C at 760 mmHg  |
| Flash Point  | 230. 8±25. 7 °C  |
| Molar Refractivity  | 109. 0±0. 3 cm 3  |
| Polarizability  | 43. 2±0. 5 10 -24 cm 3  |
| Surface Tension  | 38. 0±3. 0 dyne/cm  |
| Molar Volume  | 350. 7±3. 0 cm 3  |

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

## Experimental Melting Point:

|  |
| --- |
| 78 °CLKT Labs[T6935]  |
| 79 °CJean-Claude Bradley Open Melting Point Dataset21463  |

## Experimental LogP:

|  |
| --- |
| 4. 337Vitas-MSTK624973  |

## Experimental Solubility:

|  |
| --- |
| 10 mM in H2OMedChem ExpressHY-B0380  |
| DMSO 50 mg/mL; Water <1 mg/mLMedChem ExpressHY-B0380  |
| Soluble in methylene chloride. LKT Labs[T6935]  |

* Miscellaneous

## Safety:

|  |
| --- |
| NoneLKT Labs[T6935]  |

## Target Organs:

|  |
| --- |
| Opioid ReceptorTargetMolT0918  |

## Bio Activity:

|  |
| --- |
| Antispasmodic agentZerenex Molecular[ZBioX-0154]  |
| GPCR/G proteinMedChem ExpressHY-B0380  |
| GPCR/G protein; Neuronal Signaling; MedChem ExpressHY-B0380  |
| NeuroscienceTargetMolT0918  |
| Opioid ReceptorMedChem ExpressHY-B0380  |
| Opioid ReceptorTargetMolT0918  |
| Trimebutine is a drug with antimuscarinic and weak mu opioid agonist effects. MedChem Express  |
| Trimebutine is a drug with antimuscarinic and weak mu opioid agonist effects.; Target: Opioid Receptor; Trimebutine is an agonist of peripheral mu, kappa and delta opiate receptors, used as spasmolytic agent for treatment of both acute and chronic abdominal pain [1]. MedChem ExpressHY-B0380  |
| Trimebutine is a drug with antimuscarinic and weak mu opioid agonist effects.; Target: Opioid Receptor; Trimebutine is an agonist of peripheral mu, kappa and delta opiate receptors, used as spasmolytic agent for treatment of both acute and chronic abdominal pain [1]. The major product from drug metabolism of trimebutine in human beings is nor-trimebutine, which comes from removal of one of the methyl groups attached to nitrogen. Trimebutine exerts its effects in part due to causing a premature activation of phase III of the migrating motor complex in the digestive tract [2, 3]. MedChem ExpressHY-B0380  |

* Gas Chromatography

## Retention Index (Kovats):

|  |
| --- |
| 2762 (estimated with error: 89)NIST Spectramainlib\_121217  |

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

|  |  |
| --- | --- |
| Density:  | 1. 1±0. 1 g/cm 3  |
| Boiling Point:  | 457. 9±34. 0 °C at 760 mmHg  |
| Vapour Pressure:  | 0. 0±1. 1 mmHg at 25°C  |
| Enthalpy of Vaporization:  | 71. 8±3. 0 kJ/mol  |
| Flash Point:  | 230. 8±25. 7 °C  |
| Index of Refraction:  | 1. 534  |
| Molar Refractivity:  | 109. 0±0. 3 cm 3  |
| #H bond acceptors:  | 6  |
| #H bond donors:  | 0  |
| #Freely Rotating Bonds:  | 10  |
| #Rule of 5 Violations:  | 0  |

|  |  |
| --- | --- |
| ACD/LogP:  | 4. 34  |
| ACD/LogD (pH 5. 5):  | 1. 99  |
| ACD/BCF (pH 5. 5):  | 7. 12  |
| ACD/KOC (pH 5. 5):  | 44. 29  |
| ACD/LogD (pH 7. 4):  | 3. 51  |
| ACD/BCF (pH 7. 4):  | 240. 32  |
| ACD/KOC (pH 7. 4):  | 1494. 89  |
| Polar Surface Area:  | 57 Å 2  |
| Polarizability:  | 43. 2±0. 5 10 -24 cm 3  |
| Surface Tension:  | 38. 0±3. 0 dyne/cm  |
| Molar Volume:  | 350. 7±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) = 3. 62Boiling Pt, Melting Pt, Vapor Pressure Estimations (MPBPWIN v1. 42): Boiling Pt (deg C): 448. 69 (Adapted Stein & Brown method)Melting Pt (deg C): 178. 43 (Mean or Weighted MP)VP(mm Hg, 25 deg C): 1. 62E-007 (Modified Grain method)MP (exp database): 79 deg CSubcooled liquid VP: 5. 3E-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): 30. 47log Kow used: 3. 62 (estimated)no-melting pt equation usedWater Sol Estimate from Fragments: Wat Sol (v1. 01 est) = 2. 9272 mg/LECOSAR Class Program (ECOSAR v0. 99h): Class(es) found: Aliphatic AminesEstersHenrys Law Constant (25 deg C) [HENRYWIN v3. 10]: Bond Method : 6. 73E-013 atm-m3/moleGroup Method: IncompleteHenrys LC [VP/WSol estimate using EPI values]: 2. 711E-009 atm-m3/moleLog Octanol-Air Partition Coefficient (25 deg C) [KOAWIN v1. 10]: Log Kow used: 3. 62 (KowWin est)Log Kaw used: -10. 560 (HenryWin est)Log Koa (KOAWIN v1. 10 estimate): 14. 180Log Koa (experimental database): NoneProbability of Rapid Biodegradation (BIOWIN v4. 10): Biowin1 (Linear Model) : 0. 8719Biowin2 (Non-Linear Model) : 0. 9979Expert Survey Biodegradation Results: Biowin3 (Ultimate Survey Model): 1. 8638 (months )Biowin4 (Primary Survey Model) : 3. 3125 (days-weeks )MITI Biodegradation Probability: Biowin5 (MITI Linear Model) : 0. 6304Biowin6 (MITI Non-Linear Model): 0. 2952Anaerobic Biodegradation Probability: Biowin7 (Anaerobic Linear Model): -0. 7424Ready 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): 7. 07E-005 Pa (5. 3E-007 mm Hg)Log Koa (Koawin est ): 14. 180Kp (particle/gas partition coef. (m3/ug)): Mackay model : 0. 0425 Octanol/air (Koa) model: 37. 2 Fraction sorbed to airborne particulates (phi): Junge-Pankow model : 0. 605 Mackay model : 0. 773 Octanol/air (Koa) model: 1 Atmospheric Oxidation (25 deg C) [AopWin v1. 92]: Hydroxyl Radicals Reaction: OVERALL OH Rate Constant = 124. 8323 E-12 cm3/molecule-secHalf-Life = 0. 086 Days (12-hr day; 1. 5E6 OH/cm3)Half-Life = 1. 028 HrsOzone Reaction: No Ozone Reaction EstimationFraction sorbed to airborne particulates (phi): 0. 689 (Junge, Mackay)Note: the sorbed fraction may be resistant to atmospheric oxidationSoil Adsorption Coefficient (PCKOCWIN v1. 66): Koc : 6. 241E+004Log Koc: 4. 795 Aqueous Base/Acid-Catalyzed Hydrolysis (25 deg C) [HYDROWIN v1. 67]: Total Kb for pH > 8 at 25 deg C : 4. 183E-002 L/mol-secKb Half-Life at pH 8: 191. 771 days Kb Half-Life at pH 7: 5. 250 years Bioaccumulation Estimates from Log Kow (BCFWIN v2. 17): Log BCF from regression-based method = 2. 084 (BCF = 121. 3)log Kow used: 3. 62 (estimated)Volatilization from Water: Henry LC: 6. 73E-013 atm-m3/mole (estimated by Bond SAR Method)Half-Life from Model River: 1. 712E+009 hours (7. 135E+007 days)Half-Life from Model Lake : 1. 868E+010 hours (7. 784E+008 days)Removal In Wastewater Treatment: Total removal: 16. 06 percentTotal biodegradation: 0. 21 percentTotal sludge adsorption: 15. 85 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 3. 76e-006 2. 06 1000 Water 9 1. 44e+003 1000 Soil 90 2. 88e+003 1000 Sediment 1. 05 1. 3e+004 0 Persistence Time: 2. 85e+003 hr

Click to predict properties on the Chemicalize site

* 1-Click Docking
* 1-Click Scaffold Hop