# Trimebutine c22h29no5 structure

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- 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

    ReceptorTargetMolT091

    8

  - **Bio Activity:**

    Antispasmodic

    agentZerenex

Molecular[ZBioX-0154]

GPCR/G

proteinMedChem

ExpressHY-B0380

GPCR/G protein;

Neuronal Signaling;

MedChem ExpressHY-

B0380

NeuroscienceTargetMolT

0918

Opioid

ReceptorMedChem

ExpressHY-B0380

Opioid

ReceptorTargetMolT091

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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

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