2-methyl-1-phenyl-2-propanol c10h14o structure

Contents

- Retention Index (Linear):

Molecular Formula	$C_{10}H_{14}O$
Average mass	150. 218 Da
Density	1. 0±0. 1 g/cm ^{3}
Boiling Point	215. 0±8. 0 °C at 760 mmHg
Flash Point	81. 1±0. 0 °C
Molar Refractivity	46. 6±0. 3 cm ^{3}
Polarizability	18. 5±0. 5 10^{-24} cm ^{3}
Surface Tension	36. 4±3. 0 dyne/cm
Molar Volume	152. 8±3. 0 cm ^{3}

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

- Predicted – ChemAxon
- Predicted – Mcule
- Experimental Physico-chemical Properties

Experimental Melting Point:

23-25 °CAlfa Aesar

24 °CJean-Claude Bradley Open Melting Point Dataset2859, 20682

23-25 °CAlfa AesarL03679

24 °CFooDBFDB008187

Experimental Boiling Point:

215 °CAlfa Aesar

214-216 °CFood and Agriculture Organization of the United Nations2-Methyl-1-phenylpropan-2-ol

215 °CAlfa

AesarL03679

1 °C / 58 mmHg (69.

8871 °C / 760

mmHg)FooDBFDB00

8187

- **Experimental Flash Point:**

23 °CTCID0783

82 °CAlfa Aesar

82 °CAlfa Aesar

82 °F (27. 7778 °C)Alfa

AesarL03679

- **Experimental Gravity:**

20 g/mLMerck Millipore4351

20 g/lMerck Millipore4351,

840096

0. 974 g/mLAlfa AesarL03679

- **Experimental Refraction Index:**

1. 514Alfa

AesarL03679

1. 514-1. 517

(Liquid)Food and Agriculture Organization of the United Nations2-Methyl-1-phenylpropan-2-ol

20

(Liquid)FooDBFDB008187

- Miscellaneous

- **Appearance:**

  Colourless to pale yellow viscous liquid or white crystalline solid; Warm, herbaceous, floral aromaFood and Agriculture Organization of the United Nations2-Methyl-1-

phenylpropan-2-ol

- **Safety:**

  22Alfa AesarL03679

  36Alfa AesarL03679

  GHS07BiosynthW-

  108935

  H302Alfa

  AesarL03679

  H302BiosynthW-

  108935

  HARMFULAlfa

  AesarL03679

  P264-P270-

  P301+P312-P330-

  P501aAlfa

  AesarL03679

  WarningAlfa

  AesarL03679

  WarningBiosynthW-

108935

WARNING: Irritates skin and eyes, harmful if swallowedAlfa AesarL03679

- Gas Chromatography

Retention Index (Kovats):

1184 (estimated with error: 41)NIST Spectramainlib_232311, replib_285185, replib_131780, replib_156522, replib_114583

1140. 9 (Program type: Isothermal; Col… (show more)umn class: Standard non-polar; Column diameter: 0. 35 mm; Column length: 40 m; Column type:

Capillary; Start T: 100 C; CAS no: 100867; Active phase: SE-30; Phase thickness: 0. 35 um; Data type: Kovats RI; Authors: Tudor, E., Temperature dependence of the retention index for perfumery compounds on a SE-30 glass capillary column. I. Linear equations, J. Chromatogr. A, 779, 1997, 287-297.)NIST Spectranist ri

1781 (Program type: Isothermal; Col… (show more)umn class: Standard polar; Column type: Capillary; Start T:

150 C; CAS no: 100867; Active phase: Carbowax 20M; Phase thickness: 0. 45 um; Data type: Kovats RI; Authors: Tudor, E.; Moldovan, D.; Zarna, N., Temperature dependence of the retention index for perfumery compounds on two carbowax-20M glass capillary columns with different film thickness. 2, Rev. Roum. Chim., 44(7), 1999, 665-675.)NIST Spectranist ri

- **Retention Index (Linear):**

  1124. 6 (Program type: Ramp; Column cl... (show

more)ass: Standard non-polar; Column diameter: 0. 25 mm; Column length: 30 m; Column type: Capillary; Heat rate: 2 K/min; Start T: 50 C; End T: 300 C; CAS no: 100867; Active phase: DB-1; Data type: Linear RI; Authors: Chang, L. P.; Sheng, L. S.; Yang, M. Z.; An, D. K., Retention index of essential oil in temperature-programmed capillary column gas chromatography, Acta Pharm. Sin., 24(11), 1989, 847-852.)NIST Spectranist ri

1126. 7 (Program

type: Ramp; Column cl... (show more)ass: Standard non-polar; Column diameter: 0. 25 mm; Column length: 30 m; Column type: Capillary; Heat rate: 2 K/min; Start T: 50 C; End T: 300 C; CAS no: 100867; Active phase: DB-1; Data type: Linear RI; Authors: Chang, L. P.; Sheng, L. S.; Yang, M. Z.; An, D. K., Retention index of essential oil in temperature-programmed capillary column gas chromatography, Acta Pharm. Sin., 24(11), 1989, 847-852.)NIST

Spectranist ri

1751. 4 (Program type: Ramp; Column cl... (show more)ass: Standard polar; Column diameter: 0. 25 mm; Column length: 30 m; Column type: Capillary; Heat rate: 2 K/min; Start T: 50 C; End T: 240 C; CAS no: 100867; Active phase: DB-Wax; Data type: Linear RI; Authors: Chang, L. P.; Sheng, L. S.; Yang, M. Z.; An, D. K., Retention index of essential oil in temperature-programmed capillary column gas chromatography, Acta Pharm. Sin.,

24(11), 1989, 847-
852.)NIST
Spectranist ri

1753. 9 (Program
type: Ramp; Column
cl... (show
more)ass: Standard
polar; Column
diameter: 0. 25 mm;
Column length: 30
m; Column type:
Capillary; Heat rate:
2 K/min; Start T: 50
C; End T: 240 C;
CAS no: 100867;
Active phase: DB-
Wax; Data type:
Linear RI; Authors:
Chang, L. P.; Sheng,
L. S.; Yang, M. Z.;
An, D. K., Retention
index of essential oil
in temperature-
programmed
capillary column gas

chromatography,

Acta Pharm. Sin.,

24(11), 1989, 847-

852.)NIST

Spectranist ri

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

Density:	1. 0±0. 1 g/cm ^{3}
Boiling Point:	215. 0±8. 0 °C at 760 mmHg
Vapour Pressure:	0. 1±0. 4 mmHg at 25°C
Enthalpy of Vaporization:	47. 7±3. 0 kJ/mol
Flash Point:	81. 1±0. 0 °C
Index of Refraction:	1. 521
Molar Refractivity:	46. 6±0. 3 cm ^{3}
#H bond acceptors:	1
#H bond donors:	1
#Freely Rotating Bonds:	2
#Rule of 5 Violations:	0

ACD/LogP:	2. 06
ACD/LogD (pH 5. 5):	2. 27
ACD/BCF (pH 5. 5):	31. 37
ACD/KOC (pH 5. 5):	410. 08
ACD/LogD (pH 7. 4):	2. 27
ACD/BCF (pH 7. 4):	31. 37
ACD/KOC (pH 7. 4):	410. 08
Polar Surface Area:	20 Å ^{2}
Polarizability:	18. 5±0. 5 10 $^{-24}$ cm ^{3}
Surface Tension:	36. 4±3. 0 dyne/cm
Molar Volume:	152. 8±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) = 2. 44Boiling Pt, Melting Pt, Vapor Pressure Estimations (MPBPWIN v1. 42): Boiling Pt (deg C): 228. 78 (Adapted Stein & Brown method)Melting Pt (deg C): 19. 44 (Mean or Weighted MP)VP(mm Hg, 25 deg C): 0. 0296 (Mean VP of Antoine & Grain methods)MP (exp database): 24 deg CBP (exp database): 215 deg CWater Solubility Estimate from Log Kow (WSKOW v1. 41): Water Solubility at 25 deg C (mg/L): 2029log Kow used: 2. 44 (estimated)no-melting pt equation usedWater Sol Estimate from Fragments: Wat Sol (v1. 01 est) = 2706. 1 mg/LECOSAR Class Program (ECOSAR v0. 99h): Class(es) found: Neutral OrganicsHenrys Law Constant (25 deg C) [HENRYWIN v3. 10]: Bond Method : 5. 09E-007 atm-m3/moleGroup Method: 2. 18E-007 atm-m3/moleHenrys LC [VP/WSol estimate using EPI values]: 2. 884E-006 atm-m3/moleLog Octanol-Air Partition

Coefficient (25 deg C) [KOAWIN v1. 10]: Log Kow used: 2. 44 (KowWin est)Log Kaw used: -4. 682 (HenryWin est)Log Koa (KOAWIN v1. 10 estimate): 7. 122Log Koa (experimental database): NoneProbability of Rapid Biodegradation (BIOWIN v4. 10): Biowin1 (Linear Model) : 0. 6749Biowin2 (Non-Linear Model) : 0. 8218Expert Survey Biodegradation Results: Biowin3 (Ultimate Survey Model): 2. 6022 (weeks-months)Biowin4 (Primary Survey Model) : 3. 4139 (days-weeks)MITI Biodegradation Probability: Biowin5 (MITI Linear Model) : 0. 3191Biowin6 (MITI Non-Linear Model): 0. 2896Anaerobic Biodegradation Probability: Biowin7 (Anaerobic Linear Model): -0. 0380Ready 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): 3. 59 Pa (0. 0269 mm Hg)Log Koa (Koawin est): 7. 122Kp (particle/gas partition coef. (m3/ug)): Mackay model : 8. 36E-007 Octanol/air (Koa) model: 3. 25E-006 Fraction sorbed to airborne particulates (phi): Junge-Pankow model : 3. 02E-005 Mackay model : 6. 69E-005 Octanol/air (Koa) model: 0. 00026 Atmospheric Oxidation (25 deg C) [AopWin v1. 92]: Hydroxyl Radicals Reaction: OVERALL OH Rate Constant = 9. 5679 E-12 cm3/molecule-secHalf-Life = 1. 118 Days (12-hr day; 1. 5E6 OH/cm3)Half-Life = 13. 415 HrsOzone Reaction: No Ozone Reaction EstimationFraction sorbed to airborne particulates (phi): 4. 86E-005 (Junge, Mackay)Note: the sorbed fraction may be resistant to atmospheric oxidationSoil Adsorption Coefficient (PCKOCWIN v1. 66): Koc : 63. 74Log Koc: 1. 804 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 = 1. 177 (BCF = 15. 03)log Kow used: 2. 44 (estimated)Volatilization from Water: Henry LC: 2. 18E-007 atm-m3/mole (estimated by Group SAR Method)Half-Life from Model River: 3293 hours (137. 2 days)Half-Life from Model Lake : 3. 603E+004 hours (1501 days)Removal In Wastewater Treatment: Total removal: 2. 95 percentTotal biodegradation: 0. 10 percentTotal sludge adsorption: 2. 84 percentTotal to Air: 0. 01 percent(using 10000 hr Bio P, A, S)Level III Fugacity Model: Mass Amount Half-Life Emissions(percent) (hr) (kg/hr)Air 0. 651 26. 8 1000 Water 21. 4 900 1000 Soil 77. 8 1. 8e+003 1000 Sediment 0. 157 8. 1e+003 0 Persistence Time: 1. 1e+003 hrLog Octanol-Water Partition Coef (SRC): Log Kow (KOWWIN v1. 67 estimate) = 2. 44Boiling Pt, Melting Pt, Vapor Pressure Estimations (MPBPWIN v1. 42): Boiling Pt (deg C): 228. 78 (Adapted Stein & Brown method)Melting Pt (deg C): 19. 44 (Mean or Weighted MP)VP(mm Hg, 25 deg C): 0. 0296 (Mean VP of Antoine & Grain methods)MP (exp database): 24 deg CBP (exp database): 215 deg CWater Solubility Estimate from Log Kow (WSKOW v1. 41): Water Solubility at 25 deg C (mg/L): 2029log Kow used: 2. 44 (estimated)no-melting pt equation usedWater Sol Estimate from Fragments: Wat Sol (v1. 01 est) = 2706. 1 mg/LECOSAR Class Program (ECOSAR v0. 99h): Class(es) found: Neutral OrganicsHenrys Law Constant (25 deg C) [HENRYWIN v3. 10]: Bond Method : 5. 09E-007 atm-m3/moleGroup Method: 2. 18E-007 atm-m3/moleHenrys LC [VP/WSol estimate using EPI values]: 2. 884E-006 atm-m3/moleLog Octanol-Air Partition Coefficient (25 deg C) [KOAWIN v1. 10]: Log Kow used: 2. 44 (KowWin est)Log Kaw used: -4. 682 (HenryWin est)Log Koa (KOAWIN v1. 10 estimate): 7. 122Log Koa (experimental database): NoneProbability of Rapid Biodegradation (BIOWIN v4. 10): Biowin1 (Linear Model) : 0. 6749Biowin2 (Non-Linear Model) : 0. 8218Expert Survey Biodegradation Results: Biowin3 (Ultimate Survey Model): 2. 6022 (weeks-months)Biowin4 (Primary Survey Model) : 3. 4139 (days-weeks)MITI Biodegradation Probability: Biowin5 (MITI Linear Model) : 0. 3191Biowin6 (MITI Non-Linear Model): 0. 2896Anaerobic Biodegradation Probability: Biowin7 (Anaerobic Linear Model): -0. 0380Ready 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): 3. 59 Pa (0. 0269 mm Hg)Log Koa (Koawin

est): 7. 122Kp (particle/gas partition coef. (m3/ug)): Mackay model : 8. 36E-007 Octanol/air (Koa) model: 3. 25E-006 Fraction sorbed to airborne particulates (phi): Junge-Pankow model : 3. 02E-005 Mackay model : 6. 69E-005 Octanol/air (Koa) model: 0. 00026 Atmospheric Oxidation (25 deg C) [AopWin v1. 92]: Hydroxyl Radicals Reaction: OVERALL OH Rate Constant = 9. 5679 E-12 cm3/molecule-secHalf-Life = 1. 118 Days (12-hr day; 1. 5E6 OH/cm3)Half-Life = 13. 415 HrsOzone Reaction: No Ozone Reaction EstimationFraction sorbed to airborne particulates (phi): 4. 86E-005 (Junge, Mackay)Note: the sorbed fraction may be resistant to atmospheric oxidationSoil Adsorption Coefficient (PCKOCWIN v1. 66): Koc : 63. 74Log Koc: 1. 804 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 = 1. 177 (BCF = 15. 03)log Kow used: 2. 44 (estimated)Volatilization from Water: Henry LC: 2. 18E-007 atm-m3/mole (estimated by Group SAR Method)Half-Life from Model River: 3293 hours (137. 2 days)Half-Life from Model Lake : 3. 603E+004 hours (1501 days)Removal In Wastewater Treatment: Total removal: 2. 95 percentTotal biodegradation: 0. 10 percentTotal sludge adsorption: 2. 84 percentTotal to Air: 0. 01 percent(using 10000 hr Bio P, A, S)Level III Fugacity Model: Mass Amount Half-Life Emissions(percent) (hr) (kg/hr)Air 0. 651 26. 8 1000 Water 21. 4 900 1000 Soil 77. 8 1. 8e+003 1000 Sediment 0. 157 8. 1e+003 0 Persistence Time: 1. 1e+003 hr

Click to predict properties on the Chemicalize site

- 1-Click Docking
- 1-Click Scaffold Hop