3-(3,5-di-tert-butyl-4-hydroxyphenyl)propanoic acid c17h26o3 structure

ASSIGN BUSTER

Contents

- Retention Index (Kovats):

Molecular Formula	$C_{17}H_{26}O_3$
Average mass	278. 387 Da
Density	1. 0±0. 1 g/cm ^{3}
Boiling Point	364. 3±37. 0 °C at 760 mmHg
Flash Point	188. 3±23. 0 °C
Molar Refractivity	80. 7±0. 3 cm ^{3}
Polarizability	32. 0±0. 5 10^{-24} cm ^{3}
Surface Tension	37. 6±3. 0 dyne/cm
Molar Volume	265. 2±3. 0 cm ^{3}

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

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

Experimental Melting Point:

172-175 °CAlfa

AesarB20412

171-172

°CAcemolAMBZ0015

172-174 °CBIONET-Key

Organics

172-174

°CLabNetworkLN00117

302

172-174 °CBIONET-Key

Organics91246, 8X-

0734

Experimental LogP:

4. 479Vitas-

MSTK501703

- **Experimental Flash Point:**

  172-175 °CAlfa

  AesarB20412

- Miscellaneous

  - **Appearance:**

    White powderNovochemy[NC-

    29528]

  - **Safety:**

    20/21/36/37/39Novoch

    emy[NC-29528]

    26-37-60Alfa

    AesarB20412

    36/37/38Alfa

    AesarB20412

    36/37/38Novochemy[N

    C-29528]

    GHS07;

    GHS09Novochemy[NC-

    29528]

H315-H319-H335Alfa

AesarB20412

H332;

H403Novochemy[NC-

29528]

IRRITANTMatrix

Scientific037428

P261-P280-

P305+P351+P338-

P304+P340-P405-

P501aAlfa

AesarB20412

P332+P313;

P305+P351+P338Novo

chemy[NC-29528]

R52/53Novochemy[NC-

29528]

WarningAlfa

AesarB20412

WarningNovochemy[NC

-29528]

WARNING: Irritates

lungs, eyes, skinAlfa

AesarB20412

WARNING: Irritates skin

and eyesAlfa

AesarB20412

- Gas Chromatography

- **Retention Index (Kovats):**

  2223 (estimated with

  error: 89)NIST

  Spectramainlib_245767

  , replib_261670

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

Density:	1. 0±0. 1 g/cm ^{3}
Boiling Point:	364. 3±37. 0 °C at 760 mmHg
Vapour Pressure:	0. 0±0. 9 mmHg at 25°C
Enthalpy of Vaporization:	64. 4±3. 0 kJ/mol
Flash Point:	188. 3±23. 0 °C

Index of Refraction:	1. 520
Molar Refractivity:	80. 7±0. 3 cm^{3}
#H bond acceptors:	3
#H bond donors:	2
#Freely Rotating Bonds:	5
#Rule of 5 Violations:	0
ACD/LogP:	4. 48
ACD/LogD (pH 5. 5):	3. 56
ACD/BCF (pH 5. 5):	174. 60
ACD/KOC (pH 5. 5):	740. 88
ACD/LogD (pH 7. 4):	1. 76
ACD/BCF (pH 7. 4):	2. 74
ACD/KOC (pH 7. 4):	11. 64
Polar Surface Area:	58 $Å^{2}$
Polarizability:	32. 0±0. 5 10^{-24} cm^{3}

Surface Tension: 37. 6±3. 0 dyne/cm

Molar Volume: 265. 2±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) = 4. 77Boiling Pt, Melting Pt, Vapor Pressure Estimations (MPBPWIN v1. 42): Boiling Pt (deg C): 396. 61 (Adapted Stein & Brown method)Melting Pt (deg C): 161. 70 (Mean or Weighted MP)VP(mm Hg, 25 deg C): 8. 5E-008 (Modified Grain method)Subcooled liquid VP: 2. 15E-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): 12. 93log Kow used: 4. 77 (estimated)no-melting pt equation usedWater Sol Estimate from Fragments: Wat Sol (v1. 01 est) = 35. 038 mg/LECOSAR Class Program (ECOSAR v0. 99h): Class(es) found: Phenols-acidHenrys Law Constant (25 deg C) [HENRYWIN v3. 10]: Bond Method : 4. 07E-011 atm-m3/moleGroup Method: 5. 11E-012 atm-m3/moleHenrys LC [VP/WSol estimate using EPI values]: 2. 408E-009 atm-m3/moleLog Octanol-Air Partition Coefficient (25 deg C) [KOAWIN v1. 10]: Log Kow used: 4. 77 (KowWin est)Log Kaw used: -8. 779 (HenryWin est)Log Koa (KOAWIN v1. 10 estimate): 13. 549Log Koa (experimental database): NoneProbability of Rapid Biodegradation (BIOWIN v4. 10): Biowin1 (Linear Model) : 0. 4903Biowin2 (Non-Linear Model) : 0. 0943Expert Survey Biodegradation Results: Biowin3 (Ultimate Survey Model): 2. 5058 (weeks-months)Biowin4 (Primary Survey Model) : 3. 4959 (days-weeks)MITI Biodegradation Probability: Biowin5 (MITI Linear Model) : 0. 2772Biowin6 (MITI Non-Linear Model): 0. 0810Anaerobic Biodegradation Probability: Biowin7 (Anaerobic Linear Model): -0. 3290Ready 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. 000287 Pa (2. 15E-006 mm Hg)Log Koa (Koawin est): 13. 549Kp (particle/gas partition coef. (m3/ug)): Mackay model : 0. 0105 Octanol/air (Koa) model: 8. 69 Fraction sorbed to airborne particulates (phi): Junge-Pankow model : 0. 274 Mackay model : 0. 456 Octanol/air (Koa) model: 0. 999 Atmospheric Oxidation (25 deg C) [AopWin v1. 92]: Hydroxyl Radicals Reaction: OVERALL OH Rate Constant = 19. 8639 E-12 cm3/molecule-secHalf-Life = 0. 538 Days (12-hr day; 1. 5E6 OH/cm3)Half-Life = 6. 462 HrsOzone Reaction: No Ozone Reaction EstimationReaction With Nitrate Radicals May Be Important! Fraction sorbed to airborne particulates (phi): 0. 365 (Junge, Mackay)Note: the sorbed fraction may be resistant to atmospheric oxidationSoil Adsorption Coefficient (PCKOCWIN v1. 66): Koc : 4151Log Koc: 3. 618 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: 4. 77 (estimated)Volatilization from Water: Henry LC: 5. 11E-012 atm-m3/mole (estimated by Group SAR Method)Half-Life from Model River: 1. 912E+008 hours (7. 965E+006 days)Half-Life from Model Lake : 2. 085E+009 hours (8. 69E+007 days)Removal In Wastewater Treatment: Total

removal: 69. 10 percentTotal biodegradation: 0. 62 percentTotal sludge adsorption: 68. 48 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 4. 88e-005 12. 9 1000 Water 9. 14 900 1000 Soil 78. 3 1. 8e+003 1000 Sediment 12. 6 8. 1e+003 0 Persistence Time: 2. 1e+003 hr

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- 1-Click Docking
- 1-Click Scaffold Hop