

# [3-(3,5-di-tert-butyl-4-hydroxyphenyl)propanoic acid c17h26o3 structure](https://assignbuster.com/3-35-di-tert-butyl-4-hydroxyphenylpropanoic-acid-c17h26o3-structure/)

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 °CLabNetworkLN00117302  |
| 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:

|  |
| --- |
| 20/21/36/37/39Novochemy[NC-29528]  |
| 26-37-60Alfa AesarB20412  |
| 36/37/38Alfa AesarB20412  |
| 36/37/38Novochemy[NC-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+P338Novochemy[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

Click to predict properties on the Chemicalize site

* 1-Click Docking
* 1-Click Scaffold Hop