

Avobenzone c₂₀h₂₂o₃ structure



Contents

- Bio Activity:

Molecular Formula	$C_{20}H_{22}O_3$
Average mass	310.387 Da
Density	$1.1 \pm 0.1 \text{ g/cm}^3$
Boiling Point	$463.6 \pm 35.0 \text{ }^\circ\text{C}$ at 760 mmHg
Flash Point	$203.1 \pm 26.0 \text{ }^\circ\text{C}$
Molar Refractivity	$90.9 \pm 0.3 \text{ cm}^3$
Polarizability	$36.1 \pm 0.5 \cdot 10^{-24} \text{ cm}^3$
Surface Tension	$38.8 \pm 3.0 \text{ dyne/cm}$
Molar Volume	$287.6 \pm 3.0 \text{ cm}^3$

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

- **Experimental Melting Point:**

82 °CTCIB3382

83.5 °CJean-Claude Bradley Open Melting Point

Dataset22751

83 °CBiosynthQ-200662

- **Experimental Flash Point:**

203 °CBiosynthQ-

200662

- **Experimental Gravity:**

203 g/mL BiosynthQ-

200662

- **Experimental Solubility:**

10 mM in DMSO MedChem ExpressHY-B0316

DMSO 62 mg/mL; Water <1 mg/mL MedChem

ExpressHY-B0316

- Predicted Physico-chemical Properties

- **Predicted Melting Point:**

82 °CTCI

82

°CTCIB3382

- Miscellaneous

- **Safety:**

- GHS09BiosynthQ-200662

- H410BiosynthQ-200662

- P273; P501BiosynthQ-
200662

- TBCSynQuest2718-1-09

- WarningBiosynthQ-
200662

- **Target Organs:**

- OthersTargetMolT0
695

- **Compound Source:**

- syntheticMicrosource[0150
4190]

- **Bio Activity:**

- Avobenzone is an oil soluble ingredient used in sunscreen products to ab

full spectrum of UVA rays and a dibenzoylmethane derivative. MedChem

Avobenzene is an oil soluble ingredient used in sunscreen products to ab

full spectrum of UVA rays and a dibenzoylmethane derivative.; Target: O

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ExpressHY-B0316

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Avobenzene is an oil soluble ingredient used in sunscreen products to ab

full spectrum of UVA rays and a dibenzoylmethane derivative. It can deg

faster in light in combination with mineral UV absorbers like zinc oxide and

titanium dioxide, though with the right coating of the mineral particles th

reaction can be reduced. A manganese doped titanium dioxide may be b

than undoped titanium dioxide to improve avobenzene's stability. It reac

minerals to form colored complexes. Manufacturers of avobenzene, like L

recommend to include a chelator to prevent this from happening. They a

recommend to avoid the inclusion of iron and ferric salts, heavy metals,

formaldehyde donors and PABA and PABA esters[1]. MedChem ExpressH

OthersMedChem ExpressHY-B0316

OthersTargetMolT0695

Predicted data is generated using the ACD/Labs Percepta Platform -

PhysChem Module

Density:	1.1 ± 0.1 g/cm ³
Boiling Point:	463.6 ± 35.0 °C at 760 mmHg
Vapour Pressure:	0.0 ± 1.1 mmHg at 25°C
Enthalpy of Vaporization:	72.5 ± 3.0 kJ/mol
Flash Point:	203.1 ± 26.0 °C
Index of Refraction:	1.545
Molar Refractivity:	90.9 ± 0.3 cm ³
#H bond acceptors:	3
#H bond donors:	0
#Freely Rotating Bonds:	6
#Rule of 5 Violations:	0
ACD/LogP:	4.81
ACD/LogD (pH 5.5):	4.64
ACD/BCF (pH 5.5):	1961.45
ACD/KOC (pH 5.5):	7914.36
ACD/LogD (pH 7.4):	4.63

ACD/BCF (pH 7. 4):	1952. 63
ACD/KOC (pH 7. 4):	7878. 78
Polar Surface Area:	43 Å ²
Polarizability:	36. 1±0. 5 10 ⁻²⁴ cm ³
Surface Tension:	38. 8±3. 0 dyne/cm
Molar Volume:	287. 6±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. 51Boiling Pt, Melting Pt, Vapor Pressure Estimations (MPBPWIN v1. 42): Boiling Pt (deg C): 409. 26 (Adapted Stein & Brown method)Melting Pt (deg C): 155. 08 (Mean or Weighted MP)VP(mm Hg, 25 deg C): 1. 36E-006 (Modified Grain method)MP (exp database): 83. 5 deg CSubcooled liquid VP: 4. 95E-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): 1. 517log Kow used: 4. 51 (estimated)no-melting pt equation usedWater Sol Estimate from Fragments: Wat Sol (v1. 01 est) = 4. 9394 mg/LECOSAR Class Program (ECOSAR v0. 99h): Class(es) found: DiketonesHenrys Law Constant (25 deg C) [HENRYWIN v3. 10]: Bond Method : 2. 00E-010 atm-m³/moleGroup Method: IncompleteHenrys LC [VP/WSol estimate using EPI values]: 3. 662E-007 atm-m³/moleLog Octanol-Air Partition Coefficient (25 deg C) [KOAWIN v1. 10]: Log Kow used: 4. 51 (KowWin est)Log Kaw used: -8. 087 (HenryWin est)Log Koa (KOAWIN v1. 10 estimate): 12. 597Log Koa (experimental database): NoneProbability of Rapid Biodegradation (BIOWIN v4. 10): Biowin1 (Linear Model) : 0. 5614Biowin2 (Non-Linear Model) : 0. 1443Expert Survey Biodegradation Results: Biowin3 (Ultimate Survey Model): 2. 1980 (months)Biowin4 (Primary Survey Model) : 3. 2792 (days-weeks)MITI Biodegradation Probability: Biowin5 (MITI Linear Model) : 0. 4038Biowin6 (MITI Non-Linear Model): 0. 1710Anaerobic Biodegradation Probability: Biowin7 (Anaerobic Linear Model): -1. 1597Ready 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. 00066 Pa (4. 95E-006 mm Hg)Log Koa (Koawin est): 12. 597Kp (particle/gas partition coef. (m³/ug)): Mackay model : 0. 00455 Octanol/air (Koa) model: 0. 971 Fraction sorbed to airborne particulates (phi): Junge-Pankow model : 0. 141 Mackay model : 0. 267 Octanol/air (Koa) model: 0. 987 Atmospheric Oxidation (25 deg C) [AopWin v1. 92]: Hydroxyl Radicals Reaction: OVERALL OH Rate Constant = 25. 3757 E-12 cm³/molecule-secHalf-Life = 0. 422 Days (12-hr day; 1. 5E6 OH/cm³)Half-Life =

5. 058 HrsOzone Reaction: No Ozone Reaction EstimationFraction sorbed to airborne particulates (ϕ): 0. 204 (Junge, Mackay)Note: the sorbed fraction may be resistant to atmospheric oxidationSoil Adsorption Coefficient (PCKOCWIN v1. 66): Koc : 1705Log Koc: 3. 232 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. 929 (BCF = 84. 9)log Kow used: 4. 51 (estimated)Volatilization from Water: Henry LC: 2E-010 atm-m³/mole (estimated by Bond SAR Method)Half-Life from Model River: 5. 158E+006 hours (2. 149E+005 days)Half-Life from Model Lake : 5. 626E+007 hours (2. 344E+006 days)Removal In Wastewater Treatment: Total removal: 56. 55 percentTotal biodegradation: 0. 53 percentTotal sludge adsorption: 56. 03 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 0. 000907 10. 1 1000 Water 7. 67 1. 44e+003 1000 Soil 84. 6 2. 88e+003 1000 Sediment 7. 75 1. 3e+004 0 Persistence Time: 3. 09e+003 hr

[Click to predict properties on the Chemicalize site](https://assignbuster.com/avobenzone-c20h22o3-structure/)