Docosahexaenoic acid c22h32o2 structure

ASSIGN BUSTER

Contents

- Retention Index (Linear):

Molecular Formula	$C_{22}H_{32}O_2$
Average mass	328. 488 Da
Density	0. 9±0. 1 g/cm ^{3}
Boiling Point	446. 7±24. 0 °C at 760 mmHg
Flash Point	343. 4±18. 0 °C
Molar Refractivity	105. 9±0. 3 cm ^{3}
Polarizability	42. 0±0. 5 10^{-24} cm^3
Surface Tension	36. 0±3. 0 dyne/cm
Molar	348. 0±3. 0 cm

Volume 3

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

Experimental Melting Point:

-44

°CIndofine[10-

2206],[10-2206]

-44

°CIndofine[10-

2206],[10-2206],

[10-2206]

Experimental Solubility:

Soluble to 100

mM in

DMSOTocris

Bioscience3687

Soluble to 100

mM in DMSO and

to 100 mM in

ethanolTocris Bioscience3687

- Miscellaneous

Bio Activity:

Endogenous omega-3 fatty acid. Acts as a selective retinoid X receptor (RXR) agonist that displays no activity at RAR, thyroid hormone receptor or the vitamin D receptor (VDR). Activates all three RXR isoforms. Also shown to inhibit A? 1-42 fibrillation and toxicity in vitro. Tocris Bioscience3687

Endogenous omega-3 fatty acid. Acts as a selective retinoid X receptor (RXR) agonist that displays no activity at RAR, thyroid hormone receptor or the vitamin D receptor (VDR). Activates all three RXRisoforms. Also shown to inhibit A? 1-42 fibrillation and toxicity in vitro. Tocris Bioscience3687

Nuclear ReceptorsTocris Bioscience3687

Retinoid X

ReceptorTocris

Bioscience3687

RXR agonistTocris

Bioscience3687

- Gas Chromatography

  - **Retention Index (Kovats):**

    2612 (estimated

    with error:

    51)NIST

    Spectramainlib_3

    33235

  - **Retention Index (Normal Alkane):**

    2501. 9 (Program

    type: Ramp;

    Column cl…

    (show more)ass:

    Semi-standard

    non-polar;

    Column diameter:

    0. 25 mm;

    Column length:

    30 m; Column

    type: Capillary;

Heat rate: 5 K/min; Start T: 130 C; End T: 250 C; CAS no: 6217545; Active phase: DB-5; Carrier gas: He; Data type: Normal alkane RI; Authors: Jalali-Heravi, M.; Vosough, M., Characterization and determination of fatty acids in fish oil using gas chromatography-mass spectrometry coupled with chemometric resolution techniques, J. Chromatogr. A, 1024, 2004, 165-

176.)NIST

Spectranist ri

- **Retention Index (Linear):**

2520. 9 (Program

type: Complex;

Column… (show

more)class: Semi-

standard non-

polar; Column

diameter: 0. 25

mm; Column

length: 30 m;

Column type:

Capillary;

Description:

Multi-step

temperature

program;

T(initial)= 60C;

T(final)= 270C;

CAS no: 6217545;

Active phase: VF-

5MS; Carrier gas:

He; Phase

thickness: 0. 25

um; Data type:

Linear RI;

Authors:

Tret’yakov, K. V.,

Retention Data.

NIST Mass

Spectrometry

Data Center.,

2007.)NIST

Spectranist ri

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

Density:	0. 9±0. 1 g/cm ^{3}
Boiling Point:	446. 7±24. 0 °C at 760 mmHg
Vapour Pressure:	0. 0±2. 3 mmHg at 25°C
Enthalpy of Vaporization:	77. 3±6. 0 kJ/mol
Flash Point:	343. 4±18. 0 °C
Index of Refraction:	1. 521
Molar Refractivity:	105. 9±0. 3 cm ^{3}
#H bond acceptors:	2

#H bond donors:	1
#Freely Rotating Bonds:	14
#Rule of 5 Violations:	1
ACD/LogP:	6. 78
ACD/LogD (pH 5. 5):	5. 20
ACD/BCF (pH 5. 5):	3070. 59
ACD/KOC (pH 5. 5):	5789. 98
ACD/LogD (pH 7. 4):	3. 39
ACD/BCF (pH 7. 4):	48. 25
ACD/KOC (pH 7. 4):	90. 98
Polar Surface Area:	37 Å ^{2}
Polarizability:	42. 0±0. 5 10 $^{-24}$ cm ^{3}
Surface Tension:	36. 0±3. 0 dyne/cm
Molar Volume:	348. 0±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) = 8. 62Boiling Pt, Melting Pt, Vapor Pressure Estimations (MPBPWIN v1. 42): Boiling Pt (deg C): 449. 90 (Adapted Stein & Brown method)Melting Pt (deg C): 164. 24 (Mean or Weighted MP)VP(mm Hg, 25 deg C): 1. 83E-008 (Modified Grain method)Subcooled liquid VP: 4. 94E-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): 0. 0009028log Kow used: 8. 62 (estimated)no-melting pt equation usedWater Sol Estimate from Fragments: Wat Sol (v1. 01 est) = 0. 0089926 mg/LECOSAR Class Program (ECOSAR v0. 99h): Class(es) found: Surfactants-anionic-acidHenrys Law Constant (25 deg C) [HENRYWIN v3. 10]: Bond Method : 7. 33E-005 atm-m3/moleGroup Method: 9. 74E-008 atm-m3/moleHenrys LC [VP/WSol estimate using EPI values]: 8. 762E-006 atm-m3/moleLog Octanol-Air Partition Coefficient (25 deg C) [KOAWIN v1. 10]: Log Kow used: 8. 62 (KowWin est)Log Kaw used: -2. 523 (HenryWin est)Log Koa (KOAWIN v1. 10 estimate): 11. 143Log Koa (experimental database): NoneProbability of Rapid Biodegradation (BIOWIN v4. 10): Biowin1 (Linear Model) : 0. 7723Biowin2 (Non-Linear Model) : 0. 6965Expert Survey Biodegradation Results: Biowin3 (Ultimate Survey Model): 3. 1362 (weeks)Biowin4 (Primary Survey Model) : 4. 0284 (days)MITI Biodegradation Probability: Biowin5 (MITI Linear Model) : 0. 3860Biowin6 (MITI Non-Linear Model): 0. 1165Anaerobic Biodegradation Probability: Biowin7 (Anaerobic Linear Model): -0. 0488Ready 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): 6. 59E-005 Pa (4. 94E-007 mm Hg)Log Koa (Koawin est): 11. 143Kp (particle/gas partition coef. (m3/ug)): Mackay model : 0. 0455 Octanol/air (Koa) model: 0. 0341 Fraction sorbed to airborne particulates (phi): Junge-Pankow model : 0. 622 Mackay model : 0. 785 Octanol/air (Koa) model: 0. 732 Atmospheric Oxidation (25 deg C) [AopWin v1. 92]: Hydroxyl Radicals Reaction: OVERALL OH Rate Constant = 346. 7017 E-12 cm3/molecule-sec [Cis-isomer]OVERALL OH Rate Constant = 392. 3017 E-12 cm3/molecule-sec [Trans-isomer]Half-Life = 22. 212 Min (12-hr day; 1. 5E6 OH/cm3) [Cis-isomer]Half-Life = 19. 631 Min (12-hr day; 1. 5E6 OH/cm3) [Trans-isomer]Ozone Reaction: OVERALL Ozone Rate Constant = 78. 000000 E-17 cm3/molecule-sec [Cis-]OVERALL Ozone Rate Constant = 120. 000000 E-17 cm3/molecule-sec [Trans-]Half-Life = 21. 157 Min (at 7E11 mol/cm3) [Cis-isomer]Half-Life = 13. 752 Min (at 7E11 mol/cm3) [Trans-isomer]Reaction With Nitrate Radicals May Be Important! Fraction sorbed to airborne particulates (phi): 0. 703 (Junge, Mackay)Note: the sorbed fraction may be resistant to atmospheric oxidationSoil Adsorption Coefficient (PCKOCWIN v1. 66): Koc : 1. 351E+005Log Koc: 5. 131 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. 000 (BCF = 10)log Kow used: 8. 62 (estimated)Volatilization from Water: Henry LC: 9. 74E-008 atm-m3/mole (estimated by Group SAR Method)Half-Life from Model River: 1. 09E+004 hours (454 days)Half-Life from Model Lake : 1. 19E+005 hours (4959 days)Removal In Wastewater Treatment: Total removal: 94. 03 percentTotal biodegradation: 0. 78 percentTotal sludge adsorption: 93. 25 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. 00914 0. 239 1000 Water 3. 75 360 1000 Soil 28. 2 720 1000 Sediment 68. 1 3. 24e+003 0 Persistence Time: 1. 24e+003 hr

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