Curcumin c21h20o6 structure

Contents

- Retention Index (Kovats):

Molecular Formula	$C_{21}H_{20}O_6$
Average mass	368. 380 Da
Density	1. 3±0. 1 g/cm ^{3}
Boiling Point	591. 4±50. 0 °C at 760 mmHg
Flash Point	208. 9±23. 6 °C
Molar Refractivity	104. 0±0. 3 cm ^{3}
Polarizability	41. 2±0. 5 10^{-24} cm ^{3}
Surface Tension	54. 3±3. 0 dyne/cm
Molar Volume	287. 9±3. 0 cm ^{3}

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

- Predicted – ChemAxon
- Predicted – Mcule
- Experimental Physico-chemical Properties
  - **Experimental Melting Point:**

    183 °CTCIC0434

    170-175 °CAlfa Aesar

    180 °COxford University Chemical Safety Data (No longer updated)More details

    183 °CLKT Labs[C8069],[C8070]

    180 °CJean-Claude Bradley Open Melting Point Dataset14753

    183 °CJean-Claude Bradley Open Melting Point Dataset25369

173 °CJean-Claude

Bradley Open Melting

Point Dataset6684

170-175 °CAlfa

AesarB21573

175 °CBiosynthQ-

200901

183

°CLabNetworkLN00193

260

183 °CIndofine[C-004],

[024739S],[NR-011]

183

°CFooDBFDB012292

- **Experimental Flash Point:**

209 °CBiosynthQ-

200901

- **Experimental Gravity:**

209 g/mLBiosynthQ-

200901

- **Experimental Solubility:**

  DMSO: 25 mg/ml ;

  ethanol: 10 mg/ml;

  water:< 0. 1 mg/ml;

  chloroformMedChem

  Expresshttp://www.

  medchemexpress.

  com/Geniposide. html,

  HY-N0005

  ethanol: 10

  mg/mLIndofine[024739

  S],[C-004],[NR-011]

  Insoluble in

  waterIndofine[024739S

  ],[C-004],[NR-011]

  Insoluble in water.

  Soluble in ethanol

  (10mg/mL), DMSO

  (74mg/mL), chloroform,

  acetone, DMF. Soluble

  in 0. 1 M NaOH to 3

  mg/mL-do not store

  more than 12 hours.

LKT Labs[C8069]

Insoluble in water.

Soluble in ethanol,

DMSO. LKT

Labs[C8070]

Soluble to 10 mM in

DMSO and to 5 mM in

ethanolTocris

Bioscience2841

- Predicted Physico-chemical Properties

  - **Predicted Melting Point:**

    183 °CJ&K

    Scientific207078

    183 °CTCI

    183 °CIndofine[C-004]

    183 °CTCIC0434

- Miscellaneous

  - **Appearance:**

    orange crystalline

    powderOxford

    University Chemical

Safety Data (No longer updated)More details

- **Stability:**

  Stable, but may be light sensitive. Incompatible with strong oxidizing agents. Oxford University Chemical Safety Data (No longer updated)More details

- **Toxicity:**

  ORL-MUS LD50 > 2000 mg kg-1, IPR-MUS LD50 1500 mg kg-1Oxford University Chemical Safety Data (No longer updated)More details

- **Safety:**

  26-36/37Alfa AesarB21573

  26-37-60Alfa

AesarB21573

36/37/38Alfa

AesarB21573

36/37/38LKT

Labs[C8070]

CAUTION: May irritate

eyes, skin, and

respiratory tractAlfa

AesarB21573

GHS07BiosynthQ-

200901

H315 H319 H335LKT

Labs[C8069],[C8070]

H315; H319;

H335BiosynthQ-

200901

H315-H319-H335Alfa

AesarB21573

IrritantSynQuest2920-

1-E1, 82529

NoneLKT Labs[C8069],

[C8070]

P261; P280;

P302+P352;

P304+P340;

P305+P351+P338;

P312BiosynthQ-200901

P261-P280-

P305+P351+P338-

P304+P340-P405-

P501aAlfa

AesarB21573

R36/37/38LKT

Labs[C8069]

Safety glasses. Do not

breathe dust. Oxford

University Chemical

Safety Data (No longer

updated)More details

WarningAlfa

AesarB21573

WarningBiosynthQ-200901

WARNING: Irritates lungs, eyes, skinAlfa AesarB21573

XiLKT Labs[C8069], [C8070]

- **Compound Source:**

  Isol. from Curcuma zedoaria (turmeric), other Curcuma spp. and other spp. Zerenex Molecular[ZBioX-0548]

- **Bio Activity:**

  Antiinflammatory agent; Zerenex Molecular[ZBioX-0548]

  Antitumor, anti-inflammatory and antioxidantTocris Bioscience2841

	Antitumor, anti-inflammatory and antioxidant agent. Downregulates expression of reactive-oxygen-generating enzymes (cyclooxygenase, lipoxygenase, iNOS), TNF?, IL-1, IL-6, PKC, EGFR, NF-? B, I? B kinaseand more. Upregulates expression of PPAR?, p53, Nrf2. Also displays antimicrobial, antidiabetic neuro- and cardioprotective properties in vivo.
Tocris Bioscience2841	Antitumor, anti-inflammatory and antioxidant agent. Downregulates expression of reactive-

oxygen-generating enzymes (cyclooxygenase, lipoxygenase, iNOS), TNF?, IL-1, IL-6, PKC, EGFR, NF-? B, I? B kinase and more. Upregulates expression of PPAR?, p53, Nrf2. Also displays antimicrobial, antidiabetic neuro- and cardioprotective properties in vivo. Tocris Bioscience2841

ApoptosisTocris Bioscience2841

Apoptosis InducersTocris Bioscience2841

Cell BiologyTocris Bioscience2841

Curcumin is a natural phenolic compound with impressive antioxidant properties. MedChem Expresshttp://www. medchemexpress. com/Geniposide. html, HY-N0005

Curcumin is a natural phenolic compound with impressive antioxidant properties. Curcumin is recently proved to exert its chemopreventive effects partly through the activation of nuclear factor (erythroid-2 related) factor 2 (Nrf2).; IC50 Value:; Target: Nrf2 Curcumin possesses chemopreventive properties against

several types of cancer, but the molecular mechanisms by which it induces apoptosis of cancer cells and inhibits cancer cell proliferation are not clearly understood. ; In vitro: curcumin induced the expression of forkhead box protein O1 (FOXO1) through activation of extracellular signal-regulated kinase 1/2 signaling. Curcumin inhibited cell proliferation, which was associated with upregulation of the cyclin-dependent kinase inhibitors, p27 and p21, and downregulation of cyclin D1 [2].

Treatment of AGS and HT-29 cells with curcumin enhanced the cleavage of procaspase-3, -7, -8 and -9. Meanwhile, curcumin induced endoplasmic reticulum (ER) stress and mitochondrial dysfunctionMedChem ExpressHY-N0005

Keap1-Nrf2MedChem ExpressHY-N0005

NF-kBMedChem ExpressHY-N0005

NF-kB; MedChem ExpressHY-N0005

- Gas Chromatography

- **Retention Index (Kovats):**

  3170 (estimated with error: 89)NIST Spectramainlib_228935

, replib_75938

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

Density:	1. 3±0. 1 g/cm ^{3}
Boiling Point:	591. 4±50. 0 °C at 760 mmHg
Vapour Pressure:	0. 0±1. 7 mmHg at 25°C
Enthalpy of Vaporization:	91. 5±3. 0 kJ/mol
Flash Point:	208. 9±23. 6 °C
Index of Refraction:	1. 643
Molar Refractivity:	104. 0±0. 3 cm ^{3}
#H bond acceptors:	6
#H bond donors:	2
#Freely Rotating Bonds:	8
#Rule of 5 Violations:	0
ACD/LogP:	2. 92
ACD/LogD (pH 5. 5):	2. 56

ACD/BCF (pH 5. 5):	52. 05
ACD/KOC (pH 5. 5):	588. 53
ACD/LogD (pH 7. 4):	2. 45
ACD/BCF (pH 7. 4):	40. 49
ACD/KOC (pH 7. 4):	457. 87
Polar Surface Area:	93 Å ^{2}
Polarizability:	41. 2±0. 5 10 $^{-24}$ cm ^{3}
Surface Tension:	54. 3±3. 0 dyne/cm
Molar Volume:	287. 9±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) = 3. 29Boiling Pt, Melting Pt, Vapor Pressure Estimations (MPBPWIN v1. 42): Boiling Pt (deg C): 521. 33 (Adapted Stein & Brown method)Melting Pt (deg C): 222. 56 (Mean or Weighted MP)VP(mm Hg, 25 deg C): 3. 08E-012 (Modified Grain method)MP (exp database): 183 deg CSubcooled liquid VP: 1. 37E-010 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): 7. 475log Kow used: 3. 29 (estimated)no-melting pt equation usedWater Sol Estimate from Fragments: Wat Sol (v1. 01 est) = 14. 554 mg/LECOSAR Class Program (ECOSAR v0. 99h): Class(es) found: DiketonesPhenolsVinyl/Allyl KetonesHenrys Law Constant (25 deg C) [HENRYWIN v3. 10]: Bond Method : 7. 04E-022 atm-m3/moleGroup Method: IncompleteHenrys LC [VP/WSol estimate using EPI values]: 1. 997E-013 atm-m3/moleLog Octanol-Air Partition Coefficient (25 deg C) [KOAWIN v1. 10]: Log Kow used: 3. 29 (KowWin est)Log Kaw used: -19. 541 (HenryWin est)Log Koa (KOAWIN v1. 10 estimate): 22. 831Log Koa (experimental database): NoneProbability of Rapid Biodegradation (BIOWIN v4. 10): Biowin1 (Linear Model) : 1. 0813Biowin2 (Non-Linear Model) : 0. 9603Expert Survey Biodegradation Results: Biowin3 (Ultimate Survey Model): 2. 3366 (weeks-months)Biowin4 (Primary Survey Model) : 3. 5054 (days-weeks)MITI

Biodegradation Probability: Biowin5 (MITI Linear Model) : 0. 4949Biowin6 (MITI Non-Linear Model): 0. 1799Anaerobic Biodegradation Probability: Biowin7 (Anaerobic Linear Model): -0. 4301Ready 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): 1. 83E-008 Pa (1. 37E-010 mm Hg)Log Koa (Koawin est): 22. 831Kp (particle/gas partition coef. (m3/ug)): Mackay model : 164 Octanol/air (Koa) model: 1. 66E+010 Fraction sorbed to airborne particulates (phi): Junge-Pankow model : 1 Mackay model : 1 Octanol/air (Koa) model: 1 Atmospheric Oxidation (25 deg C) [AopWin v1. 92]: Hydroxyl Radicals Reaction: OVERALL OH Rate Constant = 158. 1909 E-12 cm3/molecule-sec [Cis-isomer]OVERALL OH Rate Constant = 171. 8709 E-12 cm3/molecule-sec [Trans-isomer]Half-Life = 0. 811 Hrs (12-hr day; 1. 5E6 OH/cm3) [Cis-isomer]Half-Life = 0. 747 Hrs (12-hr day; 1. 5E6 OH/cm3) [Trans-isomer]Ozone Reaction: OVERALL Ozone Rate Constant = 2. 100000 E-17 cm3/molecule-sec [Cis-]OVERALL Ozone Rate Constant = 4. 200000 E-17 cm3/molecule-sec [Trans-]Half-Life = 13. 097 Hrs (at 7E11 mol/cm3) [Cis-isomer]Half-Life = 6. 549 Hrs (at 7E11 mol/cm3) [Trans-isomer]Reaction With Nitrate Radicals May Be Important! Fraction sorbed to airborne particulates (phi): 1 (Junge, Mackay)Note: the sorbed fraction may be resistant to atmospheric oxidationSoil Adsorption Coefficient (PCKOCWIN v1. 66): Koc : 5161Log Koc: 3. 713 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. 831 (BCF = 67. 73)log Kow used: 3. 29 (estimated)Volatilization from Water: Henry LC: 7. 04E-022 atm-m3/mole (estimated by Bond SAR Method)Half-Life from Model River: 1. 596E+018 hours (6. 651E+016 days)Half-Life from Model Lake : 1. 741E+019 hours (7. 256E+017 days)Removal In Wastewater Treatment: Total removal: 9. 07 percentTotal biodegradation: 0. 15 percentTotal sludge adsorption: 8. 91 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 1. 72e-011 1. 44 1000 Water 12 900 1000 Soil 87. 5 1. 8e+003 1000 Sediment 0. 53 8. 1e+003 0 Persistence Time: 1. 82e+003 hr

Click to predict properties on the Chemicalize site

- 1-Click Docking
- 1-Click Scaffold Hop