

# [Curcumin c21h20o6 structure](https://assignbuster.com/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| 180 °COxford University Chemical Safety Data (No longer updated)More details |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 °CLabNetworkLN00193260 |
| 183 °CIndofine[C-004],[024739S],[NR-011] |
| 183 °CFooDBFDB012292 |

## Experimental Flash Point:

|  |
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| 209 °CBiosynthQ-200901 |

## Experimental Gravity:

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| --- |
| 209 g/mLBiosynthQ-200901 |

## Experimental Solubility:

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| 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[024739S],[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:

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| 183 °CJ&K Scientific207078 |
| 183 °CTCI |
| 183 °CIndofine[C-004] |
| 183 °CTCIC0434 |

* Miscellaneous

## Appearance:

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| orange crystalline powderOxford University Chemical Safety Data (No longer updated)More details |

## Stability:

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 Oxford University Chemical Safety Data (No longer updated)More details |

## Toxicity:

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| --- |
| 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:

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

## Bio Activity:

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| 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):

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| --- |
| 3170 (estimated with error: 89)NIST Spectramainlib\_228935, replib\_75938 |

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

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| --- | --- |
| 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 |

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| --- | --- |
| 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

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* 1-Click Scaffold Hop