Ellagic acid c14h6o8 structure

Contents

Molecular Formula	$C_{14}H_6O_8$
Average mass	302. 193 Da
Density	2. 1±0. 1 g/cm ^{3}
Boiling Point	796. 5±60. 0 °C at 760 mmHg
Flash Point	310. 1±26. 4 °C
Molar Refractivity	67. 7±0. 3 cm ^{3}
Polarizability	26. 9±0. 5 10 $^{-24}$ cm ^{3}
Surface Tension	140. 4±3. 0 dyne/cm
Molar Volume	146. 2±3. 0 cm ^{3}

- **Lambda Max:**

  366FooDBFDB0125

  75

- Experimental Physico-chemical Properties

- **Experimental Melting Point:**

  450 °C (Decomposes)Alfa Aesar

  450 °C (Decomposes)Alfa AesarA15722

  300 °CLKT Labs[E4444]

  450 °CJean-Claude Bradley Open Melting Point Dataset28062

  450 °CBiosynthW-202834

  300 °C (Decomposes)LabNetworkLN00196863

  350 °CIndofine[E-001]

  360 °CFooDBFDB012575

- **Experimental Boiling Point:**

  796. 5 °CBiosynthW-202834

- **Experimental Flash Point:**

  310. 11 °CBiosynthW-

202834

- **Experimental Gravity:**

  310. 11 g/mLBiosynthW-

  202834

- **Experimental Solubility:**

  1 M NaOH: 10 mg/mL, dark greenIndofine[E-001]

  DMSO < 10 mg/mlMedChem ExpressHY-B0183

  DMSO: 30mg/mLMedChem ExpressHY-B0183

  Soluble to 0. 65 mM in ethanolTocris Bioscience3058

  Very slightly soluble in water. Soluble in 1 N NaOH (10mg/mL). LKT Labs[E4444]

- Predicted Physico-chemical Properties

  - **Predicted Melting Point:**

    350 °CIndofine[E-

    001]

- Miscellaneous

  - **Appearance:**

    cream to light yellow crystalline solidOxford University Chemical Safety D

longer updated)More details

tan to grayIndofine[E-001]

- **Stability:**

  Stable. Combustible. Incompatible withstrong oxidizing agents. Oxford U

  Chemical Safety Data (No longer updated)More details

- **Safety:**

  26-37Alfa AesarA15722

  36/37/38Alfa AesarA15722

  GHS07BiosynthW-202834

  H315 H319 H335LKT Labs[E4444]

  H315; H319; H335BiosynthW-202834

  P261; P305+P351+P338BiosynthW-202834

  R36/37/38LKT Labs[E4444]

  Safety glasses. Oxford University Chemical Safety Data (No longer updated)More details

  WarningBiosynthW-202834

  WARNING: Irreversible damage risk, protect skin/eyes/lungs. Alfa

AesarA15722

XiLKT Labs[E4444]

- **Target Organs:**

  Casein Kinase inhibitor; Carbonic anhydrase inhibitor; PKA inhibitor; PKC

  SMO inhibitorTargetMolT0465

- **Chemical Class:**

  aromaticMicrosource[0150

  2245]

- **Drug Status:**

  INNMicrosource[015022

  45]

- **Compound Source:**

  widely distributed in higher

  plantsMicrosource[01502245]

- **Bio Activity:**

  Casein Kinase 2Tocris Bioscience3058

  Cell Cycle/DNA DamageMedChem ExpressHY-B0183

  Cell Cycle/DNA Damage; MedChem ExpressHY-B0183

CK2MedChem ExpressHY-B0183

Ellagic Acid is a cell permeable and strong casein kinase 2 (CK2) inhibito
20 nM) which acts as a potent antioxidant and anti-mutagenic. MedChem

Ellagic Acid is a cell permeable and strong casein kinase 2 (CK2) inhibito
20 nM) which acts as a potent antioxidant and anti-mutagenic.; Target: C
Ellagic acid is a natural phenol antioxidant found in numerous fruits and
vegetables. MedChem ExpressHY-B0183

Ellagic Acid is a cell permeable and strong casein kinase 2 (CK2) inhibito
20 nM) which acts as a potent antioxidant and anti-mutagenic.; Target:
CK2Ellagic acid is a natural phenol antioxidant found in numerous fruits a
vegetables. The antiproliferative and antioxidant properties of ellagic aci
spurred preliminary research into the potential health benefits of ellagic
consumption. Ellagic acid is the dilactone of hexahydroxydiphenic acid. F
produce ellagic acid from hydrolysis of tannins such as ellagitannin and g
Ellagic acid has antiproliferative and antioxidant properties in a number o
vitro and small-animal models. The antiproliferative properties of ellagic
may be due to its ability to directly inhibit the DNA binding of certain
carcinogens, including nitrosamines and polycyclic aromatic hydrocarbon
with other polyphenol antioxidants, ellagic acid has a chemoprotective ef
cellular models by reducing oxidative stress. MedChem ExpressHY-B0183

Enzyme; Metabolism; Cell Cycle/CheckpointTargetMolT0465

EnzymesTocris Bioscience3058

KinasesTocris Bioscience3058

Selective inhibitor of CK2. Also inhibits glutathione S-transferaseTocris Bioscience3058

Selective, ATP-competitive inhibitor of casein kinase 2 (CK2) (IC50 values 2900, 3500, 4300 and 9400 nM for CK2, Lyn, PKA, Syk and FGR respectiv Exhibits antioxidant, antitumor and anticarcinogenic activity and also inh glutathione S-transferase. Tocris Bioscience3058

Selective, ATP-competitive inhibitor of casein kinase 2 (CK2) (IC50 values 2900, 3500, 4300 and 9400 nM for CK2, Lyn, PKA, Syk and FGR respectiv Exhibits antioxidant, antitumor and anticarcinogenic activity and also inh glutathione S-transferase. Tocris Bioscience3058

SYK, Casein kinase II; CA; PKA; PKC; SMOTargetMolT0465

- Gas Chromatography

- **Retention Index (Kovats):**

  3070 (estimated with error: 174)NIST Spectramainlib_235205

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

Density:	2. 1±0. 1 g/cm ^{3}
Boiling Point:	796. 5±60. 0 °C at 760 mmHg

Vapour Pressure:	0. 0±2. 9 mmHg at 25°C
Enthalpy of Vaporization:	119. 9±3. 0 kJ/mol
Flash Point:	310. 1±26. 4 °C
Index of Refraction:	1. 895
Molar Refractivity:	67. 7±0. 3 cm^3
#H bond acceptors:	8
#H bond donors:	4
#Freely Rotating Bonds:	0
#Rule of 5 Violations:	0
ACD/LogP:	0. 52
ACD/LogD (pH 5. 5):	0. 83
ACD/BCF (pH 5. 5):	1. 71
ACD/KOC (pH 5. 5):	32. 22
ACD/LogD (pH 7. 4):	-2. 08
ACD/BCF (pH 7. 4):	1. 00
ACD/KOC (pH 7. 4):	1. 00

Polar Surface Area:	134 Å ^{2}
Polarizability:	26. 9±0. 5 10 $^{-24}$ cm ^{3}
Surface Tension:	140. 4±3. 0 dyne/cm
Molar Volume:	146. 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) = -2. 05Boiling Pt, Melting Pt, Vapor Pressure Estimations (MPBPWIN v1. 42): Boiling Pt (deg C): 593. 63 (Adapted Stein & Brown method)Melting Pt (deg C): 256. 33 (Mean or Weighted MP)VP(mm Hg, 25 deg C): 2. 81E-015 (Modified Grain method)Subcooled liquid VP: 9. 41E-013 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. 964e+005log Kow used: -2. 05 (estimated)no-melting pt equation usedWater Sol Estimate from Fragments: Wat Sol (v1. 01 est) = 7. 0721 mg/LECOSAR Class Program (ECOSAR v0. 99h): Class(es) found: EstersPhenolsHenrys Law Constant (25 deg C) [HENRYWIN v3. 10]: Bond Method : 5. 67E-024 atm-m3/moleGroup Method: IncompleteHenrys LC [VP/WSol estimate using EPI values]: 5. 689E-021 atm-m3/moleLog Octanol-Air Partition Coefficient (25 deg C) [KOAWIN v1. 10]: Log Kow used: -2. 05 (KowWin est)Log Kaw used: -21. 635 (HenryWin est)Log Koa (KOAWIN v1. 10 estimate): 19. 585Log Koa (experimental database): NoneProbability of Rapid Biodegradation (BIOWIN v4. 10): Biowin1 (Linear Model) : 1. 4153Biowin2 (Non-Linear Model) : 1. 0000Expert Survey Biodegradation Results: Biowin3 (Ultimate Survey Model): 3. 0373 (weeks)Biowin4 (Primary Survey Model) : 4. 0284 (days)MITI Biodegradation Probability: Biowin5 (MITI Linear Model) : 0. 7739Biowin6 (MITI Non-Linear Model): 0. 7084Anaerobic Biodegradation Probability: Biowin7 (Anaerobic Linear Model): 1. 3118Ready Biodegradability Prediction: YESHydrocarbon Biodegradation (BioHCwin v1. 01): Structure incompatible with current estimation method! Sorption to aerosols (25 Dec C)[AEROWIN v1. 00]: Vapor pressure (liquid/subcooled): 1. 25E-010 Pa (9. 41E-013 mm Hg)Log Koa (Koawin est): 19. 585Kp (particle/gas partition coef. (m3/ug)): Mackay model : 2. 39E+004 Octanol/air (Koa) model: 9. 44E+006 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 = 14. 8105 E-12 cm3/molecule-secHalf-Life = 0. 722 Days (12-hr day; 1. 5E6 OH/cm3)Half-Life = 8. 666 HrsOzone Reaction: No Ozone Reaction EstimationReaction 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 : 3418Log Koc: 3. 534 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: -2. 05 (estimated)Volatilization from Water: Henry LC: 5. 67E-024 atm-

m3/mole (estimated by Bond SAR Method)Half-Life from Model River: 1. 795E+020 hours (7. 479E+018 days)Half-Life from Model Lake : 1. 958E+021 hours (8. 159E+019 days)Removal In Wastewater Treatment: Total removal: 1. 85 percentTotal biodegradation: 0. 09 percentTotal sludge adsorption: 1. 75 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 2. 21e-010 17. 3 1000 Water 39 360 1000 Soil 60. 9 720 1000 Sediment 0. 0713 3. 24e+003 0 Persistence Time: 579 hr

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