

# [Rottlerin c30h28o8 structure](https://assignbuster.com/rottlerin-c30h28o8-structure/)

Contents

* Bio Activity:

|  |  |
| --- | --- |
| Molecular Formula | C 30 H 28 O 8 |
| Average mass | 516. 539 Da |
| Density | 1. 4±0. 1 g/cm 3 |
| Boiling Point | 800. 4±65. 0 °C at 760 mmHg |
| Flash Point | 266. 0±27. 8 °C |
| Molar Refractivity | 143. 4±0. 3 cm 3 |
| Polarizability | 56. 8±0. 5 10 -24 cm 3 |
| Surface Tension | 67. 4±3. 0 dyne/cm |
| Molar Volume | 378. 8±3. 0 cm 3 |

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

## Experimental Melting Point:

|  |
| --- |
| 200 °CIndofine[027309] |
| 212 °CJean-Claude Bradley Open Melting Point Dataset25595 |
| 200 °CIndofine[027309],[027309] |

## Experimental Solubility:

|  |
| --- |
| Soluble to 2 mM in ethanol and to 100 mM in DMSOTocris Bioscience1610 |
| Soluble to 2 mM in ethanol with gentle warming and to 100 mM in DMSOTocris Bioscience1610 |
| Soluble to 2 mM in ethanol with gentle warming and to 20 mM in DMSOTocris Bioscience1610 |

* Miscellaneous

## Bio Activity:

|  |
| --- |
| EnzymesTocris Bioscience1610 |
| KinasesTocris Bioscience1610 |
| Originally reported to inhibit PKC isoforms. Also reported to inhibit CAM kinase III. However, recently shown to inhibit a wide range of protein kinases, and most potently to inhibit PRAK and MAPKAP-K2 (IC50 values are 1. 9 and 5 ? M respectively). Also shown to act as a direct mitochondrial uncoupler. Thought to stimulate autophagy by targeting upstream mTORC1 control pathways. Tocris Bioscience1610 |
| Originally reported to inhibit PKC isoforms. Also reported to inhibit CAM kinase III. However, recently shown to inhibit a wide range of protein kinases, and most potently to inhibit PRAK and MAPKAP-K2 (IC50 values are 1. 9 and 5 ? M respectively). Also shown to act as a direct mitochondrial uncoupler. Thought to stimulate autophagy by targeting upstream mTORC1 control pathways. Tocris Bioscience1610 |
| Protein Kinase CTocris Bioscience1610 |
| Reported PKC? inhibitorTocris Bioscience1610 |

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

|  |  |
| --- | --- |
| Density: | 1. 4±0. 1 g/cm 3 |
| Boiling Point: | 800. 4±65. 0 °C at 760 mmHg |
| Vapour Pressure: | 0. 0±2. 9 mmHg at 25°C |
| Enthalpy of Vaporization: | 120. 4±3. 0 kJ/mol |
| Flash Point: | 266. 0±27. 8 °C |
| Index of Refraction: | 1. 682 |
| Molar Refractivity: | 143. 4±0. 3 cm 3 |
| #H bond acceptors: | 8 |
| #H bond donors: | 5 |
| #Freely Rotating Bonds: | 6 |
| #Rule of 5 Violations: | 3 |

|  |  |
| --- | --- |
| ACD/LogP: | 8. 66 |
| ACD/LogD (pH 5. 5): | 6. 79 |
| ACD/BCF (pH 5. 5): | 83308. 73 |
| ACD/KOC (pH 5. 5): | 113419. 69 |
| ACD/LogD (pH 7. 4): | 5. 84 |
| ACD/BCF (pH 7. 4): | 9376. 03 |
| ACD/KOC (pH 7. 4): | 12764. 89 |
| Polar Surface Area: | 145 Å 2 |
| Polarizability: | 56. 8±0. 5 10 -24 cm 3 |
| Surface Tension: | 67. 4±3. 0 dyne/cm |
| Molar Volume: | 378. 8±3. 0 cm 3 |

Click to predict properties on the Chemicalize site