

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

Contents

* Bio Activity:

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| --- | --- |
| 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:

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| --- |
| 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:

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| --- |
| 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  |
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| 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