

Rottlerin c30h28o8 structure



Contents

- Bio Activity:

Molecular C₃₀ H₂₈ O

Formula 8

Average
mass 516. 539 Da

Density 1. 4±0. 1
g/cm³

800. 4±65.

Boiling Point 0 °C at 760
mmHg

Flash Point 266. 0±27.
8 °C

Molar 143. 4±0. 3

Refractivity cm³

Polarizabilit 56. 8±0. 5

y 10⁻²⁴ cm³

Surface 67. 4±3. 0

Tension dyne/cm

Molar 378. 8±3. 0

Volume cm³

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

- **Experimental Melting Point:**

200

°CIndofine[0

27309]

212 °CJean-

Claude

Bradley

Open Melting

Point

Dataset2559

5

200

°CIndofine[0

27309],

[027309]

- **Experimental Solubility:**

Soluble to 2

mM in
ethanol and
to 100 mM in
DMSO Tocris
Bioscience16
10

Soluble to 2
mM in
ethanol with
gentle
warming and
to 100 mM in
DMSO Tocris
Bioscience16
10

Soluble to 2
mM in
ethanol with
gentle
warming and
to 20 mM in
DMSO Tocris
Bioscience16

10

- Miscellaneous

- **Bio Activity:**

EnzymesTocr

is

Bioscience16

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KinasesTocri

s

Bioscience16

10

Originally

reported to

inhibit PKC

isoforms.

Also reported

to inhibit

CAM kinase

III. However,

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and MAPKAP-
K2 (IC50
values are 1.
9 and 5 ? M
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. Also shown
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direct
mitochondria
I uncoupler.
Thought to
stimulate
autophagy
by targeting
upstream
mTORC1
control
pathways.
Tocris
Bioscience16
10

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 mitochondria

I uncoupler.

Thought to

stimulate

autophagy

by targeting

upstream

mTORC1

control

pathways.

Tocris

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Protein

Kinase

CTocris

Bioscience16

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Reported

PKC?

inhibitorTocri

s

Bioscience16

10

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