

2H,8H-Benzo[1,2-b:3,4-b']dipyran-2-one, 8,8-dimethyl-

Other names:

Amyrolin

Seselin

2H-1-Benzopyran-6-acrylic acid, 5-hydroxy-2,2-dimethyl-, «delta»-lactone

Inchi:

InChI=1S/C14H12O3/c1-14(2)8-7-10-11(17-14)5-3-9-4-6-12(15)16-13(9)10/h3-8H,1-2H3

InchiKey:

QUVCQYQEIOLHFZ-UHFFFAOYSA-N

Formula:

C14H12O3

SMILES:

CC1(C)C=Cc2c(ccc3ccc(=O)oc23)O1

Mol. weight [g/mol]:

228.24

CAS:

523-59-1

Physical Properties

Property code	Value	Unit	Source
log10ws	-8.22		Crippen Method
logp	2.977		Crippen Method
mcvol	167.350	ml/mol	McGowan Method
rinpol	2022.90		NIST Webbook
rinpol	2022.90		NIST Webbook
rinpol	2101.00		NIST Webbook
rinpol	2085.00		NIST Webbook
rinpol	2101.00		NIST Webbook

Sources

McGowan Method:

<http://link.springer.com/article/10.1007/BF02311772>

NIST Webbook:

<http://webbook.nist.gov/cgi/cbook.cgi?ID=C523591&Units=SI>

Crippen Method:

<http://pubs.acs.org/doi/abs/10.1021/ci9903071>

Crippen Method:

https://www.chemeo.com/doc/models/crippen_log10ws

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
rinpol: Non-polar retention indices

Latest version available from:

<https://www.cheméo.com/cid/82-538-4/2H-8H-Benzo-1-2-b-3-4-b-dipyran-2-one-8-8-dimethyl.pdf>

Generated by Cheméo on 2024-04-20 04:13:46.152761266 +0000 UTC m=+15875675.073338579.

Cheméo (<https://www.cheméo.com>) is the biggest free database of chemical and physical data for the process industry.