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/ci990307l

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