

2H-Furo[2,3-h]-1-benzopyran-2-one, 8-(1-methylethenyl)-

Other names: 2H-Furo[2,3-h]-1-benzopyran-2-one, 8-isopropenyl-

Oroselone

5'-Isopropenylangelicin

8-(Prop-1-en-2-yl)-2H-furo[2,3-h]chromen-2-one

Inchi:

InChI=1S/C14H10O3/c1-8(2)12-7-10-11(16-12)5-3-9-4-6-13(15)17-14(9)10/h3-7H,1H2,2

InchiKey:

FQCPXIJRWHRHIP-UHFFFAOYSA-N

Formula:

C14H10O3

SMILES:

C=C(C)c1cc2c(ccc3ccc(=O)oc32)o1

Mol. weight [g/mol]:

226.23

CAS:

1760-27-6

Physical Properties

Property code	Value	Unit	Source
log10ws	-13.21		Crippen Method
logp	3.572		Crippen Method
mcvol	163.050	ml/mol	McGowan Method
rinpol	2149.30		NIST Webbook
rinpol	2149.30		NIST Webbook

Sources

McGowan Method:

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

NIST Webbook:

<http://webbook.nist.gov/cgi/cbook.cgi?ID=C1760276&Units=SI>

Crippen Method:

<http://pubs.acs.org/doi/abs/10.1021/ci990307I>

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

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