7H-furo[3,2-g][1]benzopyran-7-one, 9-[(3-methyl-2-butenyl)oxy]-

Other names: 5-Benzofuranacrylic acid, 6-hydroxy-7-((3-methyl-2-butenyl)oxy)-, «delta»-lactone
7H-Furo[3,2-g][1]benzopyran-7-one, 9-[(3-methyl-2-buten-1-yl)oxy]-
8-Isopentenyloxypsoralene
9-((3-methylbut-2-en-1-yl)oxy)-7H-furo[3,2-g]chromen-7-one
9-(3-Methylbut-2-enyloxy)furo(3,2-g)chromen-7-one
9-(3-methylbut-2-enyloxy)-7H-furo[3,2-g]chromen-7-one
9-[(3-Methylbut-2-enyl)oxy]-7H-furo[3,2-g][1]benzopyran-7-one
9-[(3-methyl-2-buten-1-yl)oxy]-7H-furo[3,2-g][1]benzopyran-7-one
Ammidin
Marmelosin
NSC 402949
Pentosalen
imperatorin

Inchi: InChI=1S/C16H14O4/c1-10(2)5-7-19-16-14-12(6-8-18-14)9-11-3-4-13(17)20-15(11)16/h3

InchiKey: OLOOJGVNMBJLLR-UHFFFAOYSA-N

Formula: C16H14O4

SMILES: CC(C)=CCOc1c2occc2cc2ccc(=O)oc12

Mol. weight [g/mol]: 270.28

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.23		Aqueous Solubility Prediction Method
logp	3.884		Crippen Method
mcvol	197.100	ml/mol	McGowan Method
rinpol	2356.00		NIST Webbook
tf	394.95	K	Cheméo Relay (1.0)

Sources

Aqueous Solubility Prediction Method: http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C482440&Units=SI

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

Solubility of Imperatorin in Ethyl Acetate, Ethanol, Methanol, n-Hexane, and Petroleum Ether from (278.2 to 318.2) K: https://www.doi.org/10.1021/je101303e

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices
tf:	Normal melting (fusion) point