7H-Furo[3,2-g][1]benzopyran-7-one, 4-[(3-methyl-2-butenyl)oxy]-

Other names: Isoimperatorin
Inchi: InChI=1S/C16H14O4/c1-10(2)5-7-19-16-11-3-4-15(17)20-14(11)9-13-12(16)6-8-18-13/h3
InchiKey: IGWDEVSBEKYORK-UHFFFAOYSA-N
Formula: C16H14O4
SMILES: CC(C)=CCOc1c2ccoc2cc2oc(=O)ccc12
Mol. weight [g/mol]: 270.28
CAS: 482-45-1

Physical Properties

Property code	Value	Unit	Source
log10ws	-13.62		Crippen Method
logp	3.884		Crippen Method
mcvol	197.100	ml/mol	McGowan Method
rinpol	2394.00		NIST Webbook
rinpol	2394.00		NIST Webbook

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C482451&Units=SI

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.chemeo.com/cid/89-621-4/7H-Furo-3-2-g-1-benzopyran-7-one-4-3-methyl-2-butenyl-oxy.pdf

Generated by Cheméo on 2024-04-29 03:19:03.127800494 +0000 UTC m=+16649992.048377806.

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