

Rutamarin

Inchi: InChI=1S/C21H24O5/c1-7-20(3,4)15-9-13-8-14-10-18(21(5,6)26-12(2)22)24-16(14)11-17
InchiKey: AWMHMGFGCLBSAY-UHFFFAOYSA-N
Formula: C₂₁H₂₄O₅
SMILES: C=CC(C)(C)c1cc2cc3c(cc2oc1=O)OC(C(C)(C)OC(C)=O)C3
Mol. weight [g/mol]: 356.41
CAS: 14882-94-1

Physical Properties

Property code	Value	Unit	Source
log10ws	-9.60		Crippen Method
logp	3.902		Crippen Method
mcvol	273.420	ml/mol	McGowan Method
rinpol	2803.50		NIST Webbook

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
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=C14882941&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

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<https://www.chemeo.com/cid/87-059-1/Rutamarin.pdf>

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