

Decursinol angelate

Inchi: InChI=1S/C19H20O5/c1-5-11(2)18(21)23-16-9-13-8-12-6-7-17(20)22-14(12)10-15(13)24
InchiKey: AGABNGOXUSXQDD-YLBKJFSISA-N
Formula: C19H20O5
SMILES: CC=C(C)C(=O)OC1Cc2cc3ccc(=O)oc3cc2OC1(C)C
Mol. weight [g/mol]: 328.36
CAS: 130848-06-5

Physical Properties

Property code	Value	Unit	Source
log10ws	-9.12		Crippen Method
logp	3.384		Crippen Method
mcvol	245.240	ml/mol	McGowan Method
rinpol	2757.00		NIST Webbook
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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=C130848065&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/32-613-5/Decursinol-angelate.pdf>

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