

Arborinine

Inchi: InChI=1S/C16H15NO4/c1-17-10-7-5-4-6-9(10)14(18)13-11(17)8-12(20-2)16(21-3)15(13)
InchiKey: ATBZZQPALSPNMF-UHFFFAOYSA-N
Formula: C16H15NO4
SMILES: COc1cc2c(c(O)c1OC)c(=O)c1ccccc1n2C
Mol. weight [g/mol]: 285.29
CAS: 489-57-6

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.58		Crippen Method
logp	2.414		Crippen Method
mcvol	207.080	ml/mol	McGowan Method
rinpol	3007.70		NIST Webbook
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Sources

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=C489576&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

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/124-807-8/Arborinine.pdf>

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