

Galipinine

Inchi: InChI=1S/C19H21NO2/c1-20-16(10-8-15-4-2-3-5-17(15)20)9-6-14-7-11-18-19(12-14)22-
InchiKey: QRYQKXWZOXSQAJ-MRXNPFEDSA-N
Formula: C19H21NO2
SMILES: CN1c2ccccc2CCC1CCc1ccc2c(c1)OCO2
Mol. weight [g/mol]: 295.38

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.85		Crippen Method
logp	3.799		Crippen Method
mcvol	231.050	ml/mol	McGowan Method
rinpola	2652.00		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=R398333&Units=SI>

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
rinpola: Non-polar retention indices

Latest version available from:

<https://www.chemeo.com/cid/10-653-5/Galipinine.pdf>

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