

Galipine

Inchi: InChI=1S/C20H21NO3/c1-22-18-11-9-14(12-20(18)24-3)8-10-15-13-19(23-2)16-6-4-5-7-
InchiKey: XYXVQWAPEQXRET-UHFFFAOYSA-N
Formula: C20H21NO3
SMILES: COc1ccc(CCc2cc(OC)c3ccccc3n2)cc1OC
Mol. weight [g/mol]: 323.39
CAS: 525-68-8

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.82		Crippen Method
logp	4.046		Crippen Method
mcvol	253.270	ml/mol	McGowan Method
rinpol	2820.00		NIST Webbook
rinpol	2820.00		NIST Webbook

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=C525688&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/62-873-4/Galipine.pdf>

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