

Glafenine

Inchi: InChI=1S/C19H17ClN2O4/c20-12-5-6-14-17(7-8-21-18(14)9-12)22-16-4-2-1-3-15(16)19(18)13-20
InchiKey: GWOFUCIGLDBNKM-UHFFFAOYSA-N
Formula: C19H17ClN2O4
SMILES: O=C(OCC(O)CO)c1ccccc1Nc1ccnc2cc(Cl)ccc12
Mol. weight [g/mol]: 372.80
CAS: 3820-67-5

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.25		Crippen Method
logp	3.142		Crippen Method
mcvol	262.970	ml/mol	McGowan Method
rinpola	2816.00		NIST Webbook
rinpola	2816.00		NIST Webbook

Sources

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C3820675&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

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

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<https://www.chemeo.com/cid/119-342-0/Glafenine.pdf>

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