

Cuspareine

Inchi: InChI=1S/C20H25NO2/c1-21-17(12-10-16-6-4-5-7-18(16)21)11-8-15-9-13-19(22-2)20(14)
InchiKey: MBIROIXKTFTFJX-QGZVFWFLSA-N
Formula: C20H25NO2
SMILES: COc1ccc(CCC2CCc3ccccc3N2C)cc1OC
Mol. weight [g/mol]: 311.42

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.88		Crippen Method
logp	4.088		Crippen Method
mcvol	256.000	ml/mol	McGowan Method
rinpol	2707.00		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=R398328&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>

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/10-876-8/Cuspareine.pdf>

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