

Tinctoine

Inchi: InChI=1S/C15H20N2O/c1-3-5-13-12-8-11(9-16(13)2)10-17-14(12)6-4-7-15(17)18/h3-4,6
InchiKey: YSPZFPABOQWUFJ-WXRRBKDZSA-N
Formula: C15H20N2O
SMILES: C=CCC1C2CC(CN1C)Cn1c2cccc1=O
Mol. weight [g/mol]: 244.33

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.52		Crippen Method
logp	1.842		Crippen Method
mcvol	198.260	ml/mol	McGowan Method
rinpol	2235.00		NIST Webbook
rinpol	2240.00		NIST Webbook
rinpol	2235.00		NIST Webbook
rinpol	2240.00		NIST Webbook
rinpol	2240.00		NIST Webbook

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=R261226&Units=SI>

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/57-246-6/Tinctoine.pdf>

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