

2-hydroxy-tacrine

Inchi: InChI=1S/C13H14N2O/c14-13-9-3-1-2-4-11(9)15-12-6-5-8(16)7-10(12)13/h1-4,8,16H,5-7
InchiKey: PYCYYSWVRAEADT-UHFFFAOYSA-N
Formula: C13H14N2O
SMILES: Nc1c2c(nc3ccccc13)CCC(O)C2
Mol. weight [g/mol]: 214.26

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.55		Crippen Method
logp	1.667		Crippen Method
mcvol	165.780	ml/mol	McGowan Method
rinpol	2130.00		NIST Webbook
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Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R398660&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>

Legend

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

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<https://www.chemeo.com/cid/27-282-9/2-hydroxy-tacrine.pdf>

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