

1-hydroxy-tacrine

Inchi: InChI=1S/C13H14N2O/c14-13-8-4-1-2-5-9(8)15-10-6-3-7-11(16)12(10)13/h1-2,4-5,11,16
InchiKey: HLVVITIAZBPKB-UHFFFAOYSA-N
Formula: C13H14N2O
SMILES: Nc1c2c(nc3ccccc13)CCCC2O
Mol. weight [g/mol]: 214.26

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.90		Crippen Method
logp	2.187		Crippen Method
mcvol	165.780	ml/mol	McGowan Method
rinpol	2134.00		NIST Webbook
rinpol	2134.00		NIST Webbook

Sources

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R398655&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>
Crippen Method: https://www.cheméo.com/doc/models/crippen_log10ws

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.cheméo.com/cid/113-798-1/1-hydroxy-tacrine.pdf>

Generated by Cheméo on 2025-12-05 22:42:47.29289478 +0000 UTC m=+4722764.822935442.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.