Tacrine

Other names:	9-Acridinamine, 1,2,3,4-tetrahydro- Acridine, 1,2,3,4-tetrahydro-9-amino- 5-Amino-6,7,8,9-tetrahydroacridine 9-Amino-1,2,3,4-tetrahydroacridine CS 12602 1,2,3,4-Tetrahydro-9-acridinamine Tetrahydroaminacrine Tetrahydroaminoacridine Tetrahydroaminocrin Tetrahydroaminocrine THA Acridine, 9-amino-1,2,3,4-tetrahydro- Acridine, 9-aminotetrahydro- 1,2,3,4-Tetrahydro-9-aminoacridine
Inchi:	InChI=1S/C13H14N2/c14-13-9-5-1-3-7-11(9)15-12-8-4-2-6-10(12)13/h1,3,5,7H,2,4,6,8H2
InchiKey:	YLJREFDVOIBQDA-UHFFFAOYSA-N
Formula:	C13H14N2
SMILES:	N=c1c2c([nH]c3ccccc13)CCCC2
Mol. weight [g/mol]:	198.26
CAS:	321-64-2

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.99		Crippen Method
logp	2.044		Crippen Method
mcvol	159.910	ml/mol	McGowan Method
rinpol	2140.00		NIST Webbook
rinpol	2165.00		NIST Webbook
rinpol	2140.00		NIST Webbook
rinpol	2160.00		NIST Webbook
rinpol	2160.00		NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C321642&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
rinpol:	Non-polar retention indices