

Acridine, 1,2,3,4,5,6,7,8-octahydro-

Other names:	Octahydroacridine 1,2,3,4,5,6,7,8-Octahydroacridine
Inchi:	InChI=1S/C13H17N/c1-3-7-12-10(5-1)9-11-6-2-4-8-13(11)14-12/h9H,1-8H2
InchiKey:	LLCXJIQXTXEQID-UHFFFAOYSA-N
Formula:	C13H17N
SMILES:	<chem>c1c2c(nc3c1CCCC3)CCCC2</chem>
Mol. weight [g/mol]:	187.28
CAS:	1658-08-8

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.24		Crippen Method
logp	2.839		Crippen Method
mcvol	158.530	ml/mol	McGowan Method
rinpol	1736.60		NIST Webbook
rinpol	1736.60		NIST Webbook
rinpol	1712.20		NIST Webbook
rinpol	1726.50		NIST Webbook
rinpol	1726.50		NIST Webbook
rinpol	1726.50		NIST Webbook
rinpol	1726.20		NIST Webbook
rinpol	1726.50		NIST Webbook
rinpol	1712.20		NIST Webbook
rinpol	1712.20		NIST Webbook
rinpol	1726.20		NIST Webbook
rinpol	1726.50		NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	448.20	K	2.30	NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1658088&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
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
rinpola:	Non-polar retention indices
tbrp:	Boiling point at reduced pressure

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