

Sophocarpine

Other names:	13,14-Didehydromatridin-15-one Matridin-15-one, 13,14-didehydro-
Inchi:	InChI=1S/C15H22N2O/c18-14-7-1-6-13-12-5-3-9-16-8-2-4-11(15(12)16)10-17(13)14/h1.7
InchiKey:	AAGFPTSOPGCENQ-UHFFFAOYSA-N
Formula:	C15H22N2O
SMILES:	O=C1C=CCC2C3CCCN4CCCC(CN12)C34
Mol. weight [g/mol]:	246.35
CAS:	6483-15-4

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.19		Crippen Method
logp	1.648		Crippen Method
mcvol	196.000	ml/mol	McGowan Method
rinpol	2281.00		NIST Webbook
rinpol	2281.00		NIST Webbook

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C6483154&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

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