

Matrine

Other names:	Matridin-15-one «alpha»-Matrine (+)-Matrine Matrene, (+)- 1H,5H,10H-Dipyrido[2,1-f:3',2',1'-ij][1,6]naphthyridin-10-one, dodecahydro-, (7aS,13aR,13bR,13cS)-
Inchi:	InChI=1S/C15H24N2O/c18-14-7-1-6-13-12-5-3-9-16-8-2-4-11(15(12)16)10-17(13)14/h11
InchiKey:	ZSBXGIUJOOQZMP-UHFFFAOYSA-N
Formula:	C15H24N2O
SMILES:	O=C1CCCC2C3CCCN4CCCC(CN12)C34
Mol. weight [g/mol]:	248.36
CAS:	519-02-8

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.34		Crippen Method
logp	1.872		Crippen Method
mcvol	200.300	ml/mol	McGowan Method
rinpol	2286.00		NIST Webbook
rinpol	2265.00		NIST Webbook
rinpol	2286.00		NIST Webbook

Sources

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=C519028&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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/93-408-6/Matrine.pdf>

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