

1H-Pyrrolizine-7-methanol, 2,3,5,7a-tetrahydro-1-hydroxy-, (1S-cis)-

Other names:	Heliotridine
Inchi:	InChI=1S/C8H13NO2/c10-5-6-1-3-9-4-2-7(11)8(6)9/h1,7-8,10-11H,2-5H2/t7-,8?/m1/s1
InchiKey:	HJSJELVDQOXCHO-GVHYBUMESA-N
Formula:	C8H13NO2
SMILES:	OCC1=CCN2CCC(O)C12
Mol. weight [g/mol]:	155.19
CAS:	520-63-8

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.14		Crippen Method
logp	-0.646		Crippen Method
mcvol	119.280	ml/mol	McGowan Method
rinpol	1445.00		NIST Webbook
rinpol	1495.00		NIST Webbook
rinpol	1447.00		NIST Webbook
rinpol	1445.00		NIST Webbook
rinpol	1447.00		NIST Webbook
rinpol	1447.00		NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C520638&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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

rinpol: Non-polar retention indices

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