2H-Quinolizine-1-methanol, octahydro-, (1R-trans)-

Other names: Lupinine
(-)-Lupinine
(1R-trans)-Octahydro-2H-quinolizine-1-methanol

Inchi: InChI=1S/C10H19NO/c12-8-9-4-3-7-11-6-2-1-5-10(9)11/h9-10,12H,1-8H2/t9-,10?/m1/s1

InchiKey: HDVAWXXJVMJBAR-YHMJZVADSA-N

Formula: C10H19NO

SMILES: OCC1CCCN2CCCCC12

Mol. weight [g/mol]: 169.26

CAS: 486-70-4

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.50		Crippen Method
logp	1.243		Crippen Method
mcvol	145.890	ml/mol	McGowan Method
rinpol	1400.00		NIST Webbook
rinpol	1405.00		NIST Webbook
rinpol	1420.00		NIST Webbook
rinpol	1424.00		NIST Webbook
rinpol	1422.00		NIST Webbook
rinpol	1420.00		NIST Webbook
rinpol	1420.00		NIST Webbook
rinpol	1420.00		NIST Webbook
rinpol	1422.00		NIST Webbook
rinpol	1424.00		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=C486704&Units=SI

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices