

Lycopodine

Other names:	Lycopodan-5-one, 15-methyl-, (15R)- Lycopodan-5-one, 16-methyl- Lycopodan-5-one, 16-methyl-, (16R)- 1,9-Ethanobenzo[i]quinolizine, lycopodan-5-one deriv.
Inchi:	InChI=1S/C16H25NO/c1-11-8-12-9-15(18)14-5-3-7-17-6-2-4-13(12)16(14,17)10-11/h11-
InchiKey:	BCZFSDNVXODRAJ-UHFFFAOYSA-N
Formula:	C16H25NO
SMILES:	<chem>CC1CC2CC(=O)C3CCCN4CCCC2C34C1</chem>
Mol. weight [g/mol]:	247.38
CAS:	466-61-5

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.09		Crippen Method
logp	2.866		Crippen Method
mcvol	204.410	ml/mol	McGowan Method
rinsol	2310.00		NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C466615&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemed.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
rinsol:	Non-polar retention indices

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