

L-Tryptophan, N-methyl-, methyl ester

Other names:	Tryptophan, N-methyl-, methyl ester, L-Indol-3-propanoic acid, «alpha»-(methylamino), methyl ester
Inchi:	InChI=1S/C13H16N2O2/c1-14-12(13(16)17-2)7-9-8-15-11-6-4-3-5-10(9)11/h3-6,8,12,14-
InchiKey:	RZRWZNRJBFLXSC-UHFFFAOYSA-N
Formula:	C13H16N2O2
SMILES:	CNC(Cc1c[nH]c2ccccc12)C(=O)OC
Mol. weight [g/mol]:	232.28
CAS:	32164-04-8

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.72		Crippen Method
logp	0.989		Crippen Method
mcvol	182.510	ml/mol	McGowan Method
rinpol	1748.00		NIST Webbook
rinpol	1748.00		NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C32164048&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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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