L-Tryptophan, N,N-dimethyl-, methyl ester

Other names:	N,N-Dimethyltryptophan methyl ester
	S-(+)-N,N-Dimethyltryptophan methyl ester
	Propanoic acid, 2-dimethylamino-3-(3-indolyl), methyl ester
Inchi:	InChI=1S/C14H18N2O2/c1-16(2)13(14(17)18-3)8-10-9-15-12-7-5-4-6-11(10)12/h4-7,9,13
InchiKey:	QFHMLRWKLHONAO-ZDUSSCGKSA-N
Formula:	C14H18N2O2
SMILES:	COC(=O)C(Cc1c[nH]c2ccccc12)N(C)C
Mol. weight [g/mol]:	246.30
CAS:	35214-77-8

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.52		Crippen Method
logp	1.332		Crippen Method
mcvol	196.600	ml/mol	McGowan Method
rinpol	2056.00		NIST Webbook
rinpol	2056.00		NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=C35214778&Units=SI

Legend

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