

Tryptophan

Other names:	DL-Tryptophan DL-«alpha»-Amino-3-indolepropionic acid DL-Tryptophan DL-Tryptophane Racemic Tryptophan Tryptophan, DL- Tryptophane (./-.)-Tryptophan NSC 13118 DL-Tryptophane
Inchi:	InChI=1S/C11H12N2O2/c12-9(11(14)15)5-7-6-13-10-4-2-1-3-8(7)10/h1-4,6,9,13H,5,12H
InchiKey:	QIVBCDIJIAJPQS-UHFFFAOYSA-N
Formula:	C11H12N2O2
SMILES:	NC(Cc1c[nH]c2ccccc12)C(=O)O
Mol. weight [g/mol]:	204.23
CAS:	54-12-6

Physical Properties

Property code	Value	Unit	Source
ie	8.43	eV	NIST Webbook
ie	7.50	eV	NIST Webbook
log10ws	-2.36		Crippen Method
logp	0.640		Crippen Method
mcvol	154.330	ml/mol	McGowan Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C54126&Units=SI

Legend

ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume

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