

L-Tryptophan, trimethylsilyl ester

Other names:	L-tryptophan, tms derivative
Inchi:	InChI=1S/C14H20N2O2Si/c1-19(2,3)18-14(17)12(15)8-10-9-16-13-7-5-4-6-11(10)13/h4-7
InchiKey:	CZNYHJUEEBXUES-UHFFFAOYSA-N
Formula:	C14H20N2O2Si
SMILES:	C[Si](C)(C)OC(=O)C(N)Cc1c[nH]c2ccccc12
Mol. weight [g/mol]:	276.41

Physical Properties

Property code	Value	Unit	Source
ie	7.89	eV	Cheméo Relay (1.0)
log10ws	-3.04		Cheméo Relay (1.0)
logp	1.934		Crippen Method
rinpol	2193.40		NIST Webbook
rinpol	2193.40		NIST Webbook
tf	400.14	K	Cheméo Relay (1.0)

Sources

Cheméo Relay (1.0, beta):

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U333270&Units=SI>

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

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Cheméo Relay (1.0):

Legend

ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
rinpol:	Non-polar retention indices
tf:	Normal melting (fusion) point

Latest version available from:

<https://www.cheméo.com/cid/13-439-0/L-Tryptophan-trimethylsilyl-ester.pdf>

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