

Threonine, MTH-TMS

Inchi:	InChI=1S/C12H26N2O2SSi2/c1-9(15-18(3,4)5)10-11(16-19(6,7)8)14(2)12(17)13-10/h9H
InchiKey:	XIWRTVDLCCYZJB-UHFFFAOYSA-N
Formula:	C12H26N2O2SSi2
SMILES:	CC(O[Si](C)(C)C)c1[nH]c(=S)n(C)c1O[Si](C)(C)C
Mol. weight [g/mol]:	318.58

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.49		Crippen Method
logp	3.727		Crippen Method
rinpol	1582.00		NIST Webbook

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R525510&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
rinpol:	Non-polar retention indices

Latest version available from:

<https://www.chemeo.com/cid/54-035-3/Threonine-MTH-TMS.pdf>

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