

Homocysteine, N,O,S-tris(trimethylsilyl)-

Other names:	Homocysteine, TMS Homocysteine, 3tms derivative
Inchi:	InChI=1S/C13H33NO2SSi3/c1-18(2,3)14-12(10-11-17-20(7,8)9)13(15)16-19(4,5)6/h12,1
InchiKey:	CLUWSVSFUBNCJV-UHFFFAOYSA-N
Formula:	C13H33NO2SSi3
SMILES:	C[Si](C)(C)NC(CCS[Si](C)(C)C)C(=O)O[Si](C)(C)C
Mol. weight [g/mol]:	351.73

Physical Properties

Property code	Value	Unit	Source
log10ws	2.54		Crippen Method
logp	4.116		Crippen Method
rinpol	1676.00		NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U141382&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
rinpol:	Non-polar retention indices

Latest version available from:

[https://www.chemeo.com/cid/56-826-3/Homocysteine-N-O-S-tris\(trimethylsilyl\).pdf](https://www.chemeo.com/cid/56-826-3/Homocysteine-N-O-S-tris(trimethylsilyl).pdf)

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