

d3-Methionine, mono-TMS

Inchi:	InChI=1S/C8H19NO2SSi/c1-12-6-5-7(9)8(10)11-13(2,3)4/h7H,5-6,9H2,1-4H3/i1D3
InchiKey:	DJSOWYSMQHQIEA-FIBGUPNXSA-N
Formula:	C8H16D3NO2SSi
SMILES:	CSCCC(N)C(=O)O[Si](C)(C)C
Mol. weight [g/mol]:	224.41

Physical Properties

Property code	Value	Unit	Source
log10ws	0.49		Crippen Method
logp	1.445		Crippen Method
rinpol	1420.00		NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R274801&Units=SI

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.cheméo.com/cid/67-469-8/d3-Methionine-mono-TMS.pdf>

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