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.chemeo.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