S-Methoxycarbonylcysteine, MTH-TMS

Inchi: InChI=1S/C10H18N2O3S2Si/c1-12-8(15-18(3,4)5)7(11-9(12)16)6-17-10(13)14-2/h6H2,1-
InchiKey: KNUINTXZPGVJDC-UHFFFAOYSA-N
Formula: C10H18N2O3S2Si
SMILES: COC(=O)SCc1[nH]c(=S)n(C)c1O[Si](C)(C)C
Mol. weight [g/mol]: 306.48

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.28		Crippen Method
logp	2.814		Crippen Method
rinpol	1546.00		NIST Webbook
rinpol	1546.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R525505&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
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