2-Oxobutanoic acid, 4-methylthio, oxime, bis-TMS

Other names: 2-Keto-4-methiol-butyric acid, oxime, TMS
Inchi: InChI=1S/C11H25NO3SSi2/c1-16-9-8-10(12-15-18(5,6)7)11(13)14-17(2,3)4/h8-9H2,1-7H
InchiKey: QHUCALKSWWWQAO-UHFFFAOYSA-N
Formula: C11H25NO3SSi2
SMILES: CSCCC(=NO[Si](C)(C)C)C(=O)O[Si](C)(C)C
Mol. weight [g/mol]: 307.56

Physical Properties

Property code	Value	Unit	Source
log10ws	1.48		Crippen Method
logp	3.325		Crippen Method
rinpol	1514.00		NIST Webbook
rinpol	1512.00		NIST Webbook
rinpol	1514.00		NIST Webbook
rinpol	1512.00		NIST Webbook
rinpol	1514.00		NIST Webbook

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R112773&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

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