Penicillamine, mono-TMS

Inchi: InChI=1S/C8H19NO2SSi/c1-8(2,12)6(9)7(10)11-13(3,4)5/h6,12H,9H2,1-5H3
InchiKey: YWSZLWBMEYZAFC-UHFFFAOYSA-N
Formula: C8H19NO2SSi
SMILES: CC(C)(S)C(N)C(=O)O[Si](C)(C)C
Mol. weight [g/mol]: 221.39

Physical Properties

Property code	Value	Unit	Source
log10ws	0.19		Crippen Method
logp	1.400		Crippen Method
rinpol	1334.00		NIST Webbook
rinpol	1366.00		NIST Webbook
rinpol	1334.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R51973&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