

Cysteic acid, TMS

Inchi: InChI=1S/C12H31NO5SSi3/c1-20(2,3)13-11(12(14)17-21(4,5)6)10-19(15,16)18-22(7,8)9
InchiKey: JYOBCXZPYMIDGX-UHFFFAOYSA-N
Formula: C12H31NO5SSi3
SMILES: C[Si](C)(C)NC(CS(=O)(=O)O[Si](C)(C)C)C(=O)O[Si](C)(C)C
Mol. weight [g/mol]: 385.70

Physical Properties

Property code	Value	Unit	Source
log10ws	3.93		Crippen Method
logp	2.339		Crippen Method
rinpol	1969.00		NIST Webbook
rinpol	1969.00		NIST Webbook

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R94517&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.chemeo.com/cid/35-098-5/Cysteic-acid-TMS.pdf>

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