

Asparagine, N,O-3TMS

Inchi: InChI=1S/C13H32N2O3Si3/c1-19(2,3)14-11(13(17)18-21(7,8)9)10-12(16)15-20(4,5)6/h1
InchiKey: XENSVLLMVLKHGJ-UHFFFAOYSA-N
Formula: C13H32N2O3Si3
SMILES: C[Si](C)(C)NC(=O)CC(N[Si](C)(C)C)C(=O)O[Si](C)(C)C
Mol. weight [g/mol]: 348.66

Physical Properties

Property code	Value	Unit	Source
log10ws	3.45		Crippen Method
logp	2.499		Crippen Method
rinpol	1686.00		NIST Webbook
rinpol	1686.00		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=R619902&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/123-901-4/Asparagine-N-O-3TMS.pdf>

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