

L-Asparagine, N,N2-bis(trimethylsilyl)-, trimethylsilyl ester

Other names: Asparagine, tris-TMS
Asparagine, 3tms derivative

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-NSHDSACASA-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

CAS: 55649-62-2

Physical Properties

Property code	Value	Unit	Source
log10ws	3.45		Crippen Method
logp	2.499		Crippen Method
rinpol	1538.00		NIST Webbook
rinpol	1543.00		NIST Webbook
rinpol	1538.00		NIST Webbook
rinpol	1543.00		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C55649622&Units=SI>

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

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

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