

asparagine, N(O,S)-isoBOC TBDMS

Inchi: InChI=1S/C15H30N2O5Si/c1-10(2)9-21-14(20)17-11(8-12(16)18)13(19)22-23(6,7)15(3,4)
InchiKey: JOEMHNMWQDVKH-LLVKDONJSA-N
Formula: C15H30N2O5Si
SMILES: CC(C)COC(=O)NC(CC(N)=O)C(=O)O[Si](C)(C)C(C)(C)C
Mol. weight [g/mol]: 346.49

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.12		Crippen Method
logp	2.161		Crippen Method
rinpol	2453.30		NIST Webbook

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R522437&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

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/39-561-6/asparagine-N-O-S-isoBOC-TBDMS.pdf>

Generated by Cheméo on 2024-05-05 14:29:04.273084048 +0000 UTC m=+17208593.193661361.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.