

aspartic acid, N(O,S)-isoBOC TBDMS

Inchi: InChI=1S/C21H43NO6Si2/c1-15(2)14-26-19(25)22-16(18(24)28-30(11,12)21(6,7)8)13-17
InchiKey: FLEOXMHDPBHKEY-MRXNPFEDSA-N
Formula: C21H43NO6Si2
SMILES: CC(C)COC(=O)NC(CC(=O)O[Si](C)(C)C(C)(C)C)C(=O)O[Si](C)(C)C(C)(C)C
Mol. weight [g/mol]: 461.74

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.34		Crippen Method
logp	5.224		Crippen Method
rinpol	2300.10		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R522442&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.cheméo.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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<https://www.cheméo.com/cid/12-132-1/aspartic-acid-N-O-S-isoBOC-TBDMS.pdf>

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