

2-Methyl aspartic acid, TMS # 1

Inchi: InChI=1S/C11H25NO4Si2/c1-11(12,10(14)16-18(5,6)7)8-9(13)15-17(2,3)4/h8,12H2,1-7H
InchiKey: MAKFNQFYUGQCAO-UHFFFAOYSA-N
Formula: C11H25NO4Si2
SMILES: CC(N)(CC(=O)O[Si](C)(C)C)C(=O)O[Si](C)(C)C
Mol. weight [g/mol]: 291.49

Physical Properties

Property code	Value	Unit	Source
log10ws	2.20		Crippen Method
logp	1.850		Crippen Method
rinpol	1392.00		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R400441&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

Latest version available from:

<https://www.chemeo.com/cid/46-510-4/2-Methyl-aspartic-acid-TMS-1.pdf>

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