

2-Methyl aspartic acid, TMS # 2

Inchi: InChI=1S/C14H33NO4Si3/c1-14(15-20(2,3)4,13(17)19-22(8,9)10)11-12(16)18-21(5,6)7/h
InchiKey: COHZKTQBUWYWOA-UHFFFAOYSA-N
Formula: C14H33NO4Si3
SMILES: CC(CC(=O)O[Si](C)(C)C)(N[Si](C)(C)C)C(=O)O[Si](C)(C)C
Mol. weight [g/mol]: 363.67

Physical Properties

Property code	Value	Unit	Source
log10ws	3.14		Crippen Method
logp	3.316		Crippen Method
rinpol	1556.00		NIST Webbook

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.cheméo.com/doc/models/crippen_log10ws
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R400456&Units=SI>

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
rinpol: Non-polar retention indices

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