

ACETYLASPARTIC ACID triTMS

Inchi: InChI=1S/C15H33NO5Si3/c1-12(19-22(2,3)4)16-13(15(18)21-24(8,9)10)11-14(17)20-23(5,6,7)
InchiKey: QVMTWZJALBUZMG-UHFFFAOYSA-N
Formula: C15H33NO5Si3
SMILES: CC(=NC(CC(=O)O[Si](C)(C)C)C(=O)O[Si](C)(C)C)O[Si](C)(C)C
Mol. weight [g/mol]: 391.68

Physical Properties

Property code	Value	Unit	Source
log10ws	3.16		Crippen Method
logp	3.771		Crippen Method
rinpol	1680.00		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R395943&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>
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/19-820-0/ACETYLASPARTIC-ACID-triTMS.pdf>

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