

1-Aminocyclohexanecarboxylic acid, ethoxycarbonylated, TBDMS

Inchi: InChI=1S/C16H31NO4Si/c1-7-20-14(19)17-16(11-9-8-10-12-16)13(18)21-22(5,6)15(2,3)
InchiKey: OVHSUXQAVKNLMV-UHFFFAOYSA-N
Formula: C16H31NO4Si
SMILES: CCOC(=O)NC1(C(=O)O[Si](C)(C)C(C)(C)C)CCCC1
Mol. weight [g/mol]: 329.51

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.47		Crippen Method
logp	3.984		Crippen Method
rinpol	1906.00		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R562886&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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