Isoleucine, ethoxycarbonylated, TBDMS

Other names: Isoleucine, ethoxycarbonylated, TBDMS
Inchi: InChI=1S/C15H31NO4Si/c1-9-11(3)12(16-14(18)19-10-2)13(17)20-21(7,8)15(4,5)6/h11-1
InchiKey: YWBPHOQYHHQYMS-UHFFFAOYSA-N
Formula: C15H31NO4Si
SMILES: CCOC(=O)NC(C(=O)O[Si](C)(C)C(C)(C)C)C(C)CC
Mol. weight [g/mol]: 317.50

Physical Properties

Property code	Value	Unit	Source
logp	3.696		Crippen Method
rinpol	1743.00		NIST Webbook
rinpol	1732.00		NIST Webbook
rinpol	1743.00		NIST Webbook

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):
Cheméo Relay (1.0, beta):
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R563923&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

logp: Octanol/Water partition coefficient
rinpol: Non-polar retention indices