

Phenylalanine, ethoxycarbonylated, TBDMS

Inchi: InChI=1S/C18H29NO4Si/c1-7-22-17(21)19-15(13-14-11-9-8-10-12-14)16(20)23-24(5,6)1
InchiKey: ZBSJUNHHUUSKGO-UHFFFAOYSA-N
Formula: C18H29NO4Si
SMILES: CCOC(=O)NC(Cc1ccccc1)C(=O)O[Si](C)(C)C(C)(C)C
Mol. weight [g/mol]: 351.51

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.52		Crippen Method
logp	3.892		Crippen Method
rinpol	2111.00		NIST Webbook
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Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R564793&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>

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/66-253-8/Phenylalanine-ethoxycarbonylated-TBDMS.pdf>

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