

Pyroglutamic acid, N-isoBOC TBDMS

Inchi: InChI=1S/C16H29NO5Si/c1-11(2)10-21-15(20)17-12(8-9-13(17)18)14(19)22-23(6,7)16(3)
InchiKey: LJMQDOAOBLEGDM-UHFFFAOYSA-N
Formula: C16H29NO5Si
SMILES: CC(C)COC(=O)N1C(=O)CCC1C(=O)O[Si](C)(C)C(C)(C)C
Mol. weight [g/mol]: 343.49

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.38		Crippen Method
logp	3.318		Crippen Method
rinpol	2053.00		NIST Webbook
rinpol	2053.00		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R260689&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
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/121-694-7/Pyroglutamic-acid-N-isoBOC-TBDMS.pdf>

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