

3-PHENYLPROPIONYLGLYCINE diTMS

Inchi: InChI=1S/C17H29NO3Si2/c1-22(2,3)20-16(13-12-15-10-8-7-9-11-15)18-14-17(19)21-23
InchiKey: YFGNJEXEONMACH-UHFFFAOYSA-N
Formula: C17H29NO3Si2
SMILES: C[Si](C)(C)OC(=O)CN=C(Cc1ccccc1)O[Si](C)(C)C
Mol. weight [g/mol]: 351.59

Physical Properties

Property code	Value	Unit	Source
log10ws	0.25		Crippen Method
logp	4.247		Crippen Method
rinpol	1950.00		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=R395903&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/67-758-7/3-PHENYLPROPIONYLGLYCINE-diTMS.pdf>

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