

N-Acetyl-L-phenylalanine, trimethylsilyl ester

Other names: Trimethylsilyl N-acetylphenylalaninate
Phe, N-acetyl, TMS
N-acetyl-L-phenylalanine, tms derivative

Inchi: InChI=1S/C14H21NO3Si/c1-11(16)15-13(14(17)18-19(2,3)4)10-12-8-6-5-7-9-12/h5-9,13

InchiKey: QNPZCOJGKNQLHK-UHFFFAOYSA-N

Formula: C₁₄H₂₁NO₃Si

SMILES: CC(=O)NC(Cc1ccccc1)C(=O)O[Si](C)(C)C

Mol. weight [g/mol]: 279.41

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.78		Crippen Method
logp	2.112		Crippen Method
rinpol	1790.00		NIST Webbook
rinpol	1816.80		NIST Webbook
rinpol	1790.00		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U332878&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/56-089-2/N-Acetyl-L-phenylalanine-trimethylsilyl-ester.pdf>

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