L-Phenylalanine, N-(trifluoroacetyl)-, trimethylsilyl ester

Other names: Trimethylsilyl 3-phenyl-2-[(trifluoroacetyl)amino]propanoate, L-Phenylalanine, N-TFA-O-TMS

Inchi: InChI=1S/C14H18F3NO3Si/c1-22(2,3)21-12(19)11(18-13(20)14(15,16)17)9-10-7-5-4-6-8

InchiKey: MRVDKKCSXVEZMU-LLVKDONJSA-N

Formula: C14H18F3NO3Si

SMILES: C[Si](C)(C)OC(=O)[C@H](Cc1ccccc1)NC(=O)C(F)(F)F

Mol. weight [g/mol]: 333.38

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.91		Cheméo Relay (1.0)
logp	2.654		Crippen Method
rinpol	1578.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C52558846&Units=SI

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

rinpol: Non-polar retention indices

Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.