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/h5-9,13H
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
hvap	87.23	kJ/mol	Cheméo Relay (1.0)
ie	8.88	eV	Cheméo Relay (1.0)
log10ws	-2.41		Cheméo Relay (1.0)
logp	2.112		Crippen Method
rinpol	1790.00		NIST Webbook
rinpol	1816.80		NIST Webbook
rinpol	1790.00		NIST Webbook
tb	582.02	K	Cheméo Relay (1.0)
tf	323.88	K	Cheméo Relay (1.0)

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U332878&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

hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point