L-Threonine, N-(trifluoroacetyl)-, trimethylsilyl ester, trifluoroacetate (ester)

Other names: L-Threonine, N,O-di(trifluoroacetyl)-, trimethylsilyl ester
Trimethylsilyl 2-[(trifluoroacetyl)amino]-3-[(trifluoroacetyl)oxy]butanoate

Inchi: InChI=1S/C11H15F6NO5Si/c1-5(22-9(21)11(15,16)17)6(7(19)23-24(2,3)4)18-8(20)10(12

InchiKey: OMNIFVPZYCPNJD-UHFFFAOYSA-N

Formula: C11H15F6NO5Si

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

Mol. weight [g/mol]: 383.32

CAS: 52558-90-4

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.72		Crippen Method
logp	1.906		Crippen Method
rinpol	1146.60		NIST Webbook

Sources

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

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C52558904&Units=SI

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

rinpol: Non-polar retention indices