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

Other names: Trimethylsilyl 3-methyl-2-[(trifluoroacetyl)amino]butanoate
N-(trifluoroacetyl)-l-valine, tms derivative

Inchi: InChI=1S/C10H18F3NO3Si/c1-6(2)7(8(15)17-18(3,4)5)14-9(16)10(11,12)13/h6-7H,1-5H3

InchiKey: KBEAYFINTJJPEE-SSDOTTSWSA-N

Formula: C10H18F3NO3Si

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

Mol. weight [g/mol]: 285.34

CAS: 52558-81-3

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.42		Crippen Method
logp	2.068		Crippen Method
rinpol	1170.00		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=C52558813&Units=SI

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

rinpol: Non-polar retention indices