

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/ci9903071
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

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<https://www.chemeo.com/cid/33-966-3/L-Valine-N-trifluoroacetyl-trimethylsilyl-ester.pdf>

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