

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

Other names:	Trimethylsilyl 3-methyl-2-[(trifluoroacetyl)amino]pentanoate L-isoleucine, n-trifluoroacetyl-, tms derivative
Inchi:	InChI=1S/C11H20F3NO3Si/c1-6-7(2)8(9(16)18-19(3,4)5)15-10(17)11(12,13)14/h7-8H,6H
InchiKey:	PJGCRYZHBTYCJIE-HTQZYQBOSA-N
Formula:	C11H20F3NO3Si
SMILES:	CCC(C)C(NC(=O)C(F)(F)F)C(=O)O[Si](C)(C)C
Mol. weight [g/mol]:	299.36
CAS:	52558-83-5

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.84		Crippen Method
logp	2.458		Crippen Method
rinpol	1242.50		NIST Webbook
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Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C52558835&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
rinpol:	Non-polar retention indices

Latest version available from:

<https://www.chemeo.com/cid/113-397-6/l-Isoleucine-N-trifluoroacetyl-trimethylsilyl-ester.pdf>

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