

I-Leucine, N-(trifluoroacetyl)-, trimethylsilyl ester

Other names: Trimethylsilyl 4-methyl-2-[(trifluoroacetyl)amino]pentanoate

N-(trifluoroacetyl)-l-leucine, tms derivative

Inchi: InChI=1S/C11H20F3NO3Si/c1-7(2)6-8(9(16)18-19(3,4)5)15-10(17)11(12,13)14/h7-8H,6H

InchiKey: ATOHQYRAXZLOPS-MRVPVSSYSA-N

Formula: C₁₁H₂₀F₃NO₃Si

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

Mol. weight [g/mol]: 299.36

CAS: 52558-82-4

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.84		Crippen Method
logp	2.458		Crippen Method
rinpol	1231.20		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=C52558824&Units=SI>

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/49-056-6/l-Leucine-N-trifluoroacetyl-trimethylsilyl-ester.pdf>

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