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: PJGCYZHBTYCJIE-YUMQZZPRSA-N
Formula: C11H20F3NO3Si
SMILES: CC[C@H](C)[C@H](NC(=O)C(F)(F)F)C(=O)O[Si](C)(C)C
Mol. weight [g/mol]: 299.36

Physical Properties

Property code	Value	Unit	Source
logp	2.458		Crippen Method
rinpol	1242.50		NIST Webbook
rinpol	1242.50		NIST Webbook

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):
Cheméo Relay (1.0, beta):
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C52558835&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

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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