Isoleucine, MTH-TMS

Inchi: InChI=1S/C11H22N2OSSi/c1-7-8(2)9-10(14-16(4,5)6)13(3)11(15)12-9/h8H,7H2,1-6H3,(H

InchiKey: UAJZXNNNFMUPRU-UHFFFAOYSA-N

Formula: C11H22N2OSSi

SMILES: CCC(C)c1[nH]c(=S)n(C)c1O[Si](C)(C)C

Mol. weight [g/mol]: 258.46

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.44		Crippen Method
logp	3.328		Crippen Method
rinpol	1649.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R525456&Units=SI

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

rinpol: Non-polar retention indices