

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

Latest version available from:

<https://www.chemeo.com/cid/22-603-7/Isoleucine-MTH-TMS.pdf>

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