

Alanine, MTH-TMS

Inchi: InChI=1S/C8H16N2OSSi/c1-6-7(11-13(3,4)5)10(2)8(12)9-6/h1-5H3,(H,9,12)
InchiKey: UTYOXUMPMZVWKX-UHFFFAOYSA-N
Formula: C8H16N2OSSi
SMILES: Cc1[nH]c(=S)n(C)c1O[Si](C)(C)C
Mol. weight [g/mol]: 216.38

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.31		Crippen Method
logp	2.123		Crippen Method
rinpol	1491.00		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=R525372&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/44-229-9/Alanine-MTH-TMS.pdf>

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