

Methyl acetyl glycine, TMS # 1

Inchi: InChI=1S/C8H17NO3Si/c1-7(10)9(2)6-8(11)12-13(3,4)5/h6H2,1-5H3
InchiKey: CRPXWVABXOTMPJ-UHFFFAOYSA-N
Formula: C8H17NO3Si
SMILES: CC(=O)N(C)CC(=O)O[Si](C)(C)C
Mol. weight [g/mol]: 203.31

Physical Properties

Property code	Value	Unit	Source
log10ws	1.57		Crippen Method
logp	0.843		Crippen Method
rinpol	1394.00		NIST Webbook
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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=R401157&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/115-831-1/Methyl-acetyl-glycine-TMS-1.pdf>

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