

2-Methylbutyryl glycine, TMS # 3

Inchi: InChI=1S/C13H29NO3Si2/c1-9-11(2)13(17-19(6,7)8)14-10-12(15)16-18(3,4)5/h14H,9-10H,11-13H2
InchiKey: YOFKTVQKBDOOJF-QBFSEMIESA-N
Formula: C13H29NO3Si2
SMILES: CCC(C)=C(NCC(=O)O[Si](C)(C)C)O[Si](C)(C)C
Mol. weight [g/mol]: 303.55

Physical Properties

Property code	Value	Unit	Source
log10ws	0.65		Crippen Method
logp	3.447		Crippen Method
rinpol	1517.00		NIST Webbook
rinpol	1517.00		NIST Webbook

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R400496&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

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/119-648-1/2-Methylbutyryl-glycine-TMS-3.pdf>

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