

2-Methyl-3-oxovaleric acid, O,O'-bis(trimethylsilyl)-

Other names: 3-Oxopentanoic acid, 2-methyl, TMS
2-Methyl-3-ketovaleric acid, di-TMS
2-Methyl-3-ketovaleric acid, enol, TMS

Inchi: InChI=1S/C12H26O3Si2/c1-9-11(14-16(3,4)5)10(2)12(13)15-17(6,7)8/h9H2,1-8H3/b11-1

InchiKey: LXAIQDVPXKOIGO-KHPPLWFESA-N

Formula: C12H26O3Si2

SMILES: CCC(O[Si](C)(C)C)=C(C)C(=O)O[Si](C)(C)C

Mol. weight [g/mol]: 274.50

Physical Properties

Property code	Value	Unit	Source
log10ws	0.75		Crippen Method
logp	3.900		Crippen Method
rinpol	1363.00		NIST Webbook
rinpol	1322.00		NIST Webbook
rinpol	1363.00		NIST Webbook
rinpol	1326.00		NIST Webbook
rinpol	1320.00		NIST Webbook
rinpol	1354.00		NIST Webbook
rinpol	1320.00		NIST Webbook
rinpol	1354.00		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U99830&Units=SI>

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307I>

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

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