

3-Trimethylsilyloxyvaleric acid, trimethylsilyl ester

Other names:	3-Trimethylsilyloxyvaleric acid, trimethylsilyl ester «beta»-Hydroxy-n-valeric acid, O,O'-bis(trimethylsilyl)- «beta»-Hydroxy-n-valeric acid di-TMS 3-Hydroxy-n-valeric acid, diTMS 3-Hydroxyvaleric acid, di-TMS 3-Hydroxyvaleric acid, TMS ether, TMS ester Pentanoic acid, 3-hydroxy, bis-TMS Pentanoic acid, 3-trimethylsilyloxy, trimethylsilyl ester 3-Hydroxyvaleric acid, TMS
Inchi:	InChI=1S/C11H26O3Si2/c1-8-10(13-15(2,3)4)9-11(12)14-16(5,6)7/h10H,8-9H2,1-7H3
InchiKey:	MXLUVLLKKRDFHE-UHFFFAOYSA-N
Formula:	C11H26O3Si2
SMILES:	CCC(CC(=O)O[Si](C)(C)C)O[Si](C)(C)C
Mol. weight [g/mol]:	262.49
CAS:	79628-62-9

Physical Properties

Property code	Value	Unit	Source
log10ws	1.41		Crippen Method
logp	3.385		Crippen Method
rinpol	1239.00		NIST Webbook
rinpol	1242.00		NIST Webbook
rinpol	1245.00		NIST Webbook
rinpol	1245.00		NIST Webbook
rinpol	1240.00		NIST Webbook
rinpol	1240.00		NIST Webbook
rinpol	1238.00		NIST Webbook
rinpol	1239.00		NIST Webbook
rinpol	1245.00		NIST Webbook
rinpol	1240.00		NIST Webbook
rinpol	1239.00		NIST Webbook
rinpol	1238.00		NIST Webbook

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.cheméo.com/doc/models/crippen_log10ws
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C79628629&Units=SI>

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
rinpol: Non-polar retention indices

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