

Butanoic acid, 2-[(trimethylsilyl)oxy]-, trimethylsilyl ester

Other names:	«alpha»-Hydroxybutyric acid (2TMS) 2-Hydroxybutyric acid, diTMS Butanoic acid, 2-hydroxy, bis-TMS Butyric acid, 2-hydroxy, di-TMS 2-Hydroxybutyric acid, TMS 2-Hydroxybutyric acid, 2tms derivative
Inchi:	InChI=1S/C10H24O3Si2/c1-8-9(12-14(2,3)4)10(11)13-15(5,6)7/h9H,8H2,1-7H3
InchiKey:	NSEFDIGCPFOEIV-UHFFFAOYSA-N
Formula:	C10H24O3Si2
SMILES:	CCC(O[Si](C)(C)C)C(=O)O[Si](C)(C)C
Mol. weight [g/mol]:	248.47
CAS:	55133-93-2

Physical Properties

Property code	Value	Unit	Source
log10ws	1.83		Crippen Method
logp	2.995		Crippen Method
rinpol	1126.00		NIST Webbook
rinpol	1137.00		NIST Webbook
rinpol	1133.00		NIST Webbook
rinpol	1129.00		NIST Webbook
rinpol	1136.00		NIST Webbook
rinpol	1136.00		NIST Webbook
rinpol	1130.00		NIST Webbook
rinpol	1133.00		NIST Webbook
rinpol	1129.00		NIST Webbook
rinpol	1130.00		NIST Webbook
rinpol	1136.00		NIST Webbook
rinpol	1157.00		NIST Webbook
rinpol	1130.00		NIST Webbook
rinpol	1129.00		NIST Webbook
rinpol	1132.00		NIST Webbook
rinpol	1130.00		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=C55133932&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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