

Propanoic acid, 2-methyl-3-[(trimethylsilyl)oxy]-, trimethylsilyl ester

Other names:	Isobutyric acid, 3-trimethylsilyloxy-trimethylsilyl ester 3-Hydroxyisobutyric acid, diTMS Isobutyric acid, 3-hydroxy, di-TMS 3-Hydroxyisobutanoic acid, bis-TMS
Inchi:	InChI=1S/C10H24O3Si2/c1-9(8-12-14(2,3)4)10(11)13-15(5,6)7/h9H,8H2,1-7H3
InchiKey:	ZLXJWFWIINAYRS-UHFFFAOYSA-N
Formula:	C10H24O3Si2
SMILES:	CC(CO[Si](C)(C)C)C(=O)O[Si](C)(C)C
Mol. weight [g/mol]:	248.47
CAS:	55530-42-2

Physical Properties

Property code	Value	Unit	Source
log10ws	2.18		Crippen Method
logp	2.852		Crippen Method
rinpol	1160.00		NIST Webbook
rinpol	1164.00		NIST Webbook
rinpol	1150.00		NIST Webbook
rinpol	1164.00		NIST Webbook
rinpol	1170.00		NIST Webbook
rinpol	1163.00		NIST Webbook
rinpol	1163.00		NIST Webbook
rinpol	1170.00		NIST Webbook
rinpol	1166.00		NIST Webbook
rinpol	1167.00		NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C55530422&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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