

2-Isopropylmalic acid, O-trimethylsilyl-, bis(trimethylsilyl) ester

Other names:	Bis(trimethylsilyl) 2-isopropyl-2-[(trimethylsilyl)oxy]succinate
Inchi:	InChI=1S/C16H36O5Si3/c1-13(2)16(21-24(9,10)11,15(18)20-23(6,7)8)12-14(17)19-22(3,
InchiKey:	NCWMZDPQUOFGKZ-UHFFFAOYSA-N
Formula:	C16H36O5Si3
SMILES:	CC(C)C(CC(=O)O[Si](C)(C)C)(O[Si](C)(C)C)C(=O)O[Si](C)(C)C
Mol. weight [g/mol]:	392.71

Physical Properties

Property code	Value	Unit	Source
log10ws	2.64		Crippen Method
logp	4.379		Crippen Method
rinpol	1562.80		NIST Webbook
rinpol	1562.80		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=U333851&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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