Butanoic acid, 2-(1-methylethyl)-2,3-bis[(trimethylsilyl)oxy]-, [2,3,5,7a-tetrahydro-1-[(trimethylsilyl)oxy]-1H-pyrr l ester, [1R-[1«alpha»,7(2R*,3S*),7a«beta»]]-

Other names:	Indicine pertrimethylsilyl ether Echinatine, triTMS
Inchi:	InChI=1S/C24H49NO5Si3/c1-18(2)24(30-33(10,11)12,19(3)28-31(4,5)6)23(26)27-17-20-
InchiKey:	BNOZTCHGOQKVFR-UHFFFAOYSA-N
Formula:	C24H49NO5Si3
SMILES:	CC(C)C(O[Si](C)(C)C)(C(=O)OCC1=CCN2CCC(O[Si](C)(C)C)C12)C(C)O[Si](C)(C)C
Mol. weight [g/mol]:	515.91
CAS:	71307-22-7

Physical Properties

Property code	Value	Unit	Source
log10ws	1.44		Crippen Method
logp	5.250		Crippen Method
rinpol	2415.00		NIST Webbook
rinpol	2415.00		NIST Webbook
rinpol	2415.00		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=C71307227&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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