trans-Aconitic acid, tris(tert-butyldimethylsilyl) ester

Other names:	Aconitic acid, (e)-, 3tbdms derivative
Inchi:	InChI=1S/C24H48O6Si3/c1-22(2,3)31(10,11)28-19(25)16-18(21(27)30-33(14,15)24(7,8)9
InchiKey:	IHNCVZAILQVPPN-FBMGVBCBSA-N
Formula:	C24H48O6Si3
SMILES:	CC(C)(C)[Si](C)(C)OC(=O)C=C(CC(=O)O[Si](C)(C)C(C)(C)C)C(=O)O[Si](C)(C)C(C)(C)C
Mol. weight [g/mol]:	516.89

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.46		Crippen Method
logp	6.948		Crippen Method
rinpol	2367.40		NIST Webbook
rinpol	2385.00		NIST Webbook

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U334019&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

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

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