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

Other names: (Z)-Aconitic acid, DMTBS
cis-Aconitic acid, TBDMS
Aconitic acid, (z)-, 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-VLGSPTGOSA-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	2368.30		NIST Webbook
rinpol	2386.00		NIST Webbook
rinpol	2389.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U333986&Units=SI

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

rinpol: Non-polar retention indices