trans-Traumatic acid, bis(tert-butyldimethylsilyl) ester

Other names: Traumatic acid, (e)-, 2tbdms derivative

Inchi: InChI=1S/C24H48O4Si2/c1-23(2,3)29(7,8)27-21(25)19-17-15-13-11-12-14-16-18-20-22(

InchiKey: XGZBHEVCUZRKHF-HTXNQAPBSA-N

Formula: C24H48O4Si2

SMILES: CC(C)(C)[Si](C)(C)OC(=O)C=CCCCCCCCCC(=O)O[Si](C)(C)C(C)(C)C

Mol. weight [g/mol]: 456.81

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.55		Crippen Method
logp	7.760		Crippen Method
rinpol	2620.30		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=U352404&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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