cis-13-Octadecenoic acid, tert-butyldimethylsilyl ester

Other names: 13-Octadecenoic acid, (z)-, tbdms derivative

Inchi: InChI=1S/C24H48O2Si/c1-7-8-9-10-11-12-13-14-15-16-17-18-19-20-21-22-23(25)26-27(

InchiKey: VHNVVKIRQGPQFX-KHPPLWFESA-N

Formula: C24H48O2Si

SMILES: CCCCC=CCCCCCCCCCCCC(=O)O[Si](C)(C)C(C)(C)C

Mol. weight [g/mol]: 396.72

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.64		Crippen Method
logp	8.572		Crippen Method
rinpol	2484.90		NIST Webbook
rinpol	2484.90		NIST Webbook

Sources

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U333587&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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