

cis-6-Octadecenoic acid, tert-butyldimethylsilyl ester

Other names: Petroselinic acid, DMTBS
Petroselinic acid, TBDMS
Petroselinic acid, 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(28)29

InchiKey: BAQHCGVJKGIVFT-ZCXUNETKSA-N

Formula: C24H48O2Si

SMILES: CCCCCCCCCC=CCCCC(=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	2460.00		NIST Webbook
rinpol	2467.00		NIST Webbook
rinpol	2454.90		NIST Webbook
rinpol	2460.00		NIST Webbook
rinpol	2454.90		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U333220&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

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