

9,12-Octadecadiynoic acid, tert-butyldimethylsilyl ester

Inchi: InChI=1S/C24H42O2Si/c1-7-8-9-10-11-12-13-14-15-16-17-18-19-20-21-22-23(25)26-27(28)29
InchiKey: ONEFLCFORGOXSV-UHFFFAOYSA-N
Formula: C24H42O2Si
SMILES: CCCCC#CCC#CCCCCCCCC(=O)O[Si](C)(C)C(C)(C)C
Mol. weight [g/mol]: 390.67

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.37		Crippen Method
logp	7.243		Crippen Method
rinpol	2557.90		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U333565&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
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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<https://www.chemeo.com/cid/37-744-5/9-12-Octadecadiynoic-acid-tert-butyldimethylsilyl-ester.pdf>

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