

cis-9-Hexadecenoic acid, tert-butyldimethylsilyl ester

Other names:	Palmitoleic acid, DMTBS Palmitoleic acid, TBDMS 9-Hexadecenoic acid, (z)-, tbdms derivative
Inchi:	InChI=1S/C22H44O2Si/c1-7-8-9-10-11-12-13-14-15-16-17-18-19-20-21(23)24-25(5,6)22
InchiKey:	VSFVIVLUCDIIB-SEYXRHQNSA-N
Formula:	C22H44O2Si
SMILES:	CCCCCCC=CCCCCCCC(=O)O[Si](C)(C)C(C)(C)C
Mol. weight [g/mol]:	368.67

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.80		Crippen Method
logp	7.792		Crippen Method
rinpol	2268.50		NIST Webbook
rinpol	2268.00		NIST Webbook
rinpol	2271.00		NIST Webbook
rinpol	2268.50		NIST Webbook
rinpol	2268.00		NIST Webbook

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U333197&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

Latest version available from:

<https://www.cheméo.com/cid/57-227-7/cis-9-Hexadecenoic-acid-tert-butyl-dimethylsilyl-ester.pdf>

Generated by Cheméo on 2024-04-26 13:51:05.34548477 +0000 UTC m=+16428714.266062088.

Cheméo (<https://www.cheméo.com>) is the biggest free database of chemical and physical data for the process industry.