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: VSFAVIVLUCDIIB-SEYXRHQNSA-N

Formula: C22H44O2Si

SMILES: CCCCCC/C=C\CCCCCCCC(=O)O[Si](C)(C)C(C)(C)C

Mol. weight [g/mol]: 368.68

Physical Properties

Property code	Value	Unit	Source
hf	-828.41	kJ/mol	Cheméo Relay (1.0)
hvap	95.59	kJ/mol	Cheméo Relay (1.0)
log10ws	-6.44		Cheméo Relay (1.0)
logp	7.792		Crippen Method
pc	832.79	kPa	Cheméo Relay (1.0, beta)
rinpol	2271.00		NIST Webbook
rinpol	2268.00		NIST Webbook
rinpol	2268.00		NIST Webbook
rinpol	2268.50		NIST Webbook
rinpol	2268.50		NIST Webbook
tb	587.21	K	Cheméo Relay (1.0)
tc	792.07	K	Cheméo Relay (1.0)
tf	253.34	K	Cheméo Relay (1.0)

Sources

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U333197&Units=SI

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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

Legend

hf:	Enthalpy of formation at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
pc:	Critical Pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point