CIS, 6-OCTADECENOIC ACID, TRIMETHYLSILYL ESTER

Other names: Petroselinic acid, tms derivative
Inchi: InChI=1S/C21H42O2Si/c1-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19-20-21(22)23-24(2,3
InchiKey: NEABEGUTEOTBEL-NXVVXOECSA-N
Formula: C21H42O2Si
SMILES: CCCCCCCCCCC/C=C\CCCCC(=O)O[Si](C)(C)C
Mol. weight [g/mol]: 354.65

Physical Properties

Property code	Value	Unit	Source
af	0.8978		Cheméo Relay (1.0)
gf	-95.40	kJ/mol	Cheméo Relay (1.0, beta)
hf	-829.43	kJ/mol	Cheméo Relay (1.0)
hvap	102.02	kJ/mol	Cheméo Relay (1.0)
ie	9.26	eV	Cheméo Relay (1.0)
log10ws	-6.54		Cheméo Relay (1.0)
logp	7.402		Crippen Method
pc	549.86	kPa	Cheméo Relay (1.0, beta)
rinpol	2209.00		NIST Webbook
rinpol	2211.00		NIST Webbook
rinpol	2211.00		NIST Webbook
tb	590.38	K	Cheméo Relay (1.0)
tc	766.12	K	Cheméo Relay (1.0)
tf	246.32	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=C96851535&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

af:	Acentric Factor
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
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