TETRACOSANOIC ACID, TRIMETHYLSILYL ESTER

Other names: Tetracosanoic acid, TMS
Lignoceric acid, tms derivative

Inchi: InChI=1S/C27H56O2Si/c1-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19-20-21-22-23-24-25

InchiKey: MFKGSZQXHZDMAM-UHFFFAOYSA-N

Formula: C27H56O2Si

SMILES: CCCCCCCCCCCCCCCCCCCCCCCC(=O)O[Si](C)(C)C

Mol. weight [g/mol]: 440.83

Physical Properties

Property code	Value	Unit	Source
af	1.1874		Cheméo Relay (1.0)
hf	-1029.65	kJ/mol	Cheméo Relay (1.0)
hvap	126.87	kJ/mol	Cheméo Relay (1.0)
ie	10.22	eV	Cheméo Relay (1.0)
log10ws	-9.02		Cheméo Relay (1.0)
logp	9.967		Crippen Method
pc	33.14	kPa	Cheméo Relay (1.0, beta)
rinpol	2829.00		NIST Webbook
rinpol	2826.80		NIST Webbook
rinpol	2835.00		NIST Webbook
rinpol	2838.00		NIST Webbook
rinpol	2848.00		NIST Webbook
rinpol	2837.00		NIST Webbook
rinpol	2850.00		NIST Webbook
rinpol	2839.00		NIST Webbook
rinpol	2835.00		NIST Webbook
tb	634.10	K	Cheméo Relay (1.0)
tc	814.19	K	Cheméo Relay (1.0)
tf	316.26	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=C74367376&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
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