Hexadecanoic acid, tert-butyldimethylsilyl ester

Other names: Hexadecanoic acid, DMTBS
Hexadecanoic acid, TBDMS
Palmitic acid, TBDMS
Palmitic acid, DMTBS
tert-Butyl(dimethyl)silyl palmitate
Palmitic acid, tbdms derivative

Inchi: InChI=1S/C22H46O2Si/c1-7-8-9-10-11-12-13-14-15-16-17-18-19-20-21(23)24-25(5,6)22

InchiKey: GPNFTJMLPUJTAA-UHFFFAOYSA-N

Formula: C22H46O2Si

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

Mol. weight [g/mol]: 370.68

CAS: 58160-87-5

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.94		Crippen Method
logp	8.016		Crippen Method
rinpol	2289.00		NIST Webbook
rinpol	2281.20		NIST Webbook
rinpol	2263.00		NIST Webbook
rinpol	2288.00		NIST Webbook
rinpol	2290.00		NIST Webbook
rinpol	2275.00		NIST Webbook
rinpol	2281.20		NIST Webbook
rinpol	2290.00		NIST Webbook
rinpol	2288.00		NIST Webbook
ripol	2370.00		NIST Webbook
ripol	2370.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C58160875&Units=SI

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

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
ripol:	Polar retention indices