

n-Pentadecanoic acid, trimethylsilyl ester

Other names:	n-Pentanoic acid, trimethylsilyl ester Pentadecanoic acid, TMS ester Pentadecanoic acid, trimethylsilyl ester Pentadecanoic acid, TMS Trimethylsilyl pentadecanoate Pentadecanoic acid, tms derivative
Inchi:	InChI=1S/C18H38O2Si/c1-5-6-7-8-9-10-11-12-13-14-15-16-17-18(19)20-21(2,3)4/h5-17H
InchiKey:	SHDTWSQDHLKGEO-UHFFFAOYSA-N
Formula:	C18H38O2Si
SMILES:	CCCCCCCCCCCCCCCC(=O)O[Si](C)(C)C
Mol. weight [g/mol]:	314.58
CAS:	74367-22-9

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.27		Crippen Method
logp	6.456		Crippen Method
rinpol	1947.00		NIST Webbook
rinpol	1942.00		NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C74367229&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

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