

Monocaprylin, bis(trimethylsilyl)- deriv.

Other names:	Monocaprylin, bis(trimethylsilyl) Octanoic acid, 2,3-bis-(OTMS) propyl ester Octanoic acid, 2,3-bis-(OTMS) propyl ester («alpha»-glyceryl caprilate)
Inchi:	InChI=1S/C17H38O4Si2/c1-8-9-10-11-12-13-17(18)19-14-16(21-23(5,6)7)15-20-22(2,3)4
InchiKey:	DJRROAREVKKRCI-UHFFFAOYSA-N
Formula:	C17H38O4Si2
SMILES:	CCCCCCCC(=O)OCC(CO[Si](C)(C)C)O[Si](C)(C)C
Mol. weight [g/mol]:	362.65
CAS:	1851-21-4

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.19		Crippen Method
logp	4.962		Crippen Method
rinpol	1851.00		NIST Webbook
rinpol	1851.00		NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1851214&Units=SI

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
rinpol:	Non-polar retention indices

Latest version available from:

<https://www.chemeo.com/cid/35-199-3/Monocaprylin-bis-trimethylsilyl-deriv.pdf>

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