

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]:	362.66

Physical Properties

Property code	Value	Unit	Source
hf	-1166.05	kJ/mol	Cheméo Relay (1.0)
hvap	74.69	kJ/mol	Cheméo Relay (1.0)
log10ws	-3.39		Cheméo Relay (1.0)
logp	4.962		Crippen Method
pc	785.43	kPa	Cheméo Relay (1.0, beta)
rinpol	1851.00		NIST Webbook
tb	577.84	K	Cheméo Relay (1.0)
tc	717.84	K	Cheméo Relay (1.0)
tf	241.92	K	Cheméo Relay (1.0)

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1851214&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	

Legend

hf:	Enthalpy of formation at standard conditions
hvac:	Enthalpy of vaporization at standard conditions
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

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