Heptanedioic acid, bis(trimethylsilyl) ester

Other names:	Pimelic acid, bis(trimethylsilyl)-, ester
	Pimelic acid (2TMS)
	Heptanedioic acid, bis-TMS ester
	Pimelic acid, bis-TMS
	Pimelic acid, diTMS
	Heptanedioic acid, 1,7-bis(trimethylsilyl) ester
	Pimelic acid (tms)
	Heptanedioic acid, TMS ester
	Pimelic acid, 2tms derivative
Inchi:	InChI=1S/C13H28O4Si2/c1-18(2,3)16-12(14)10-8-7-9-11-13(15)17-19(4,5)6/h7-11H2,1-6
InchiKey:	VOLKRTUGJXKFMI-UHFFFAOYSA-N
Formula:	C13H28O4Si2
SMILES:	C[Si](C)(C)OC(=O)CCCCCC(=O)O[Si](C)(C)C
Mol. weight [g/mol]:	304.53
CAS:	55530-58-0

Physical Properties

Property code	Value	Unit	Source
log10ws	0.91		Crippen Method
logp	3.693		Crippen Method
rinpol	1591.00		NIST Webbook
rinpol	1608.00		NIST Webbook
rinpol	1611.00		NIST Webbook
rinpol	1594.00		NIST Webbook
rinpol	1610.00		NIST Webbook
rinpol	1593.00		NIST Webbook
rinpol	1592.00		NIST Webbook
rinpol	1591.00		NIST Webbook
rinpol	1610.00		NIST Webbook
rinpol	1612.00		NIST Webbook
rinpol	1604.00		NIST Webbook
rinpol	1592.00		NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C55530580&Units=SI

Legend

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