Octanedioic acid, bis(trimethylsilyl) ester

Other names:	Suberic acid trimethylsilyl ester
	Suberic acid (2TMS)
	Suberic acid, di(trimethylsilyl)ester
	Bis(trimethylsilyl) suberate
	Octanedioic acid, diTMS
	Octanedioic acid, bis-TMS
	Octanedioic acid, bisTMS ester
	Suberate, TMS
	Suberic acid, bis-TMS
	Suberic acid, diTMS
	Octanedioic acid, 1,8-bis(trimethylsilyl) ester
	Suberic acid (tms)
	3-Methylsuberic acid, di-TMS
	Octanedioic acid, TMS
	Octanedioic acid, TMS ester
	Octanedioic acid, 3-hydroxy, TMS
	Suberic acid, 2tms derivative
Inchi:	InChI=1S/C14H30O4Si2/c1-19(2,3)17-13(15)11-9-7-8-10-12-14(16)18-20(4,5)6/h7-12H2
InchiKey:	LWDVKORSFQXPHL-UHFFFAOYSA-N
Formula:	C14H30O4Si2
SMILES:	C[Si](C)(C)OC(=O)CCCCCCC(=O)O[Si](C)(C)C
Mol. weight [g/mol]:	318.56
CAS:	43199-48-0

Physical Properties

Property code	Value	Unit	Source
log10ws	0.49		Crippen Method
logp	4.083		Crippen Method
rinpol	1691.00		NIST Webbook
rinpol	1682.00		NIST Webbook
rinpol	1702.00		NIST Webbook
rinpol	1689.00		NIST Webbook
rinpol	1692.00		NIST Webbook
rinpol	1707.00		NIST Webbook
rinpol	1691.00		NIST Webbook
rinpol	1710.00		NIST Webbook
rinpol	1691.00		NIST Webbook

rinpol	1687.00	NIST Webbook
rinpol	1730.00	NIST Webbook
rinpol	1710.00	NIST Webbook
rinpol	1718.00	NIST Webbook
rinpol	1710.00	NIST Webbook
rinpol	1707.00	NIST Webbook
rinpol	1694.00	NIST Webbook
rinpol	1687.00	NIST Webbook
rinpol	1702.00	NIST Webbook
rinpol	1692.00	NIST Webbook
rinpol	1710.00	NIST Webbook
rinpol	1702.00	NIST Webbook
rinpol	1691.00	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=C43199480&Units=SI

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

rinpol: Non-polar retention indices