

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)CCCCC(=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	1702.00		NIST Webbook
rinpol	1730.00		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

rropol	1710.00	NIST Webbook
rropol	1691.00	NIST Webbook
rropol	1687.00	NIST Webbook
rropol	1691.00	NIST Webbook
rropol	1710.00	NIST Webbook
rropol	1718.00	NIST Webbook
rropol	1710.00	NIST Webbook
rropol	1707.00	NIST Webbook
rropol	1694.00	NIST Webbook
rropol	1687.00	NIST Webbook
rropol	1702.00	NIST Webbook
rropol	1692.00	NIST Webbook
rropol	1710.00	NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.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
rropol:	Non-polar retention indices

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