

2-Hexenedioic acid, bis(trimethylsilyl) ester, (E)-

Other names:	trans-2-Hexenedioic acid, TMS
Inchi:	InChI=1S/C12H24O4Si2/c1-17(2,3)15-11(13)9-7-8-10-12(14)16-18(4,5)6/h7,9H,8,10H2,1
InchiKey:	BVXJLSYCPJDQEM-VQHVLOKHSA-N
Formula:	C12H24O4Si2
SMILES:	C[Si](C)(C)OC(=O)C=CCCC(=O)O[Si](C)(C)C
Mol. weight [g/mol]:	288.49
CAS:	55494-10-5

Physical Properties

Property code	Value	Unit	Source
log10ws	1.47		Crippen Method
logp	3.079		Crippen Method
rinpol	1539.00		NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C55494105&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

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

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<https://www.chemeo.com/cid/76-888-3/2-Hexenedioic-acid-bis-trimethylsilyl-ester-E.pdf>

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