

2-Pentenedioic acid, 2-[(trimethylsilyl)oxy]-, bis(trimethylsilyl) ester

Other names:	2-Ketoglutaric acid, tri-TMS 2-Ketoglutaric acid, tris(trimethylsilyl)- deriv. Bis(trimethylsilyl) 2-[(trimethylsilyl)oxy]-2-pentenedioate 2-Ketoglutaric acid, enol, tri-TMS 2-Pentenedioic acid, 2-[(trimethylsilyl)oxy]-, 1,5-bis(trimethylsilyl) ester
Inchi:	InChI=1S/C14H30O5Si3/c1-20(2,3)17-12(14(16)19-22(7,8)9)10-11-13(15)18-21(4,5)6/h1
InchiKey:	TZIXNQWQHKLOGH-BENRWUELSA-N
Formula:	C14H30O5Si3
SMILES:	<chem>C[Si](C)(C)OC(=O)CC=C(O[Si](C)(C)C)C(=O)O[Si](C)(C)C</chem>
Mol. weight [g/mol]:	362.64
CAS:	55590-97-1

Physical Properties

Property code	Value	Unit	Source
log10ws	3.00		Crippen Method
logp	3.868		Crippen Method
rinsol	1622.00		NIST Webbook
rinsol	1622.00		NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemo.com/doc/models/crippen_log10ws
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C55590971&Units=SI

Legend

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

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