

2-Pentenedioic acid, bis(trimethylsilyl) ester

Other names:	Glutaconic acid, di(trimethylsilyl) ester Bis(trimethylsilyl) 2-pentenedioate Glutaconic acid, bis-TMS Glutaconic acid, di-TMS 2-Pentenedioic acid, 2tms derivative
Inchi:	InChI=1S/C11H22O4Si2/c1-16(2,3)14-10(12)8-7-9-11(13)15-17(4,5)6/h7-8H,9H2,1-6H3/
InchiKey:	XYCDBRYVUTZVCR-BQYQJAHWSA-N
Formula:	C11H22O4Si2
SMILES:	C[Si](C)(C)OC(=O)C=CCC(=O)O[Si](C)(C)C
Mol. weight [g/mol]:	274.46
CAS:	55255-43-1

Physical Properties

Property code	Value	Unit	Source
log10ws	1.89		Crippen Method
logp	2.689		Crippen Method
rinpol	1448.00		NIST Webbook
rinpol	1453.00		NIST Webbook
rinpol	1456.00		NIST Webbook
rinpol	1460.00		NIST Webbook
rinpol	1448.00		NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C55255431&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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

Latest version available from:

<https://www.cheméo.com/cid/13-138-4/2-Pentenedioic-acid-bis-trimethylsilyl-ester.pdf>

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