

Methylmaleic acid, bis(trimethylsilyl) ester

Other names:	2-Butenedioic acid, 2-methyl-, bis(trimethylsilyl) ester Mesaconic acid, bis(trimethylsilyl) ester Methylmaleic acid, 2tms derivative
Inchi:	InChI=1S/C11H22O4Si2/c1-9(11(13)15-17(5,6)7)8-10(12)14-16(2,3)4/h8H,1-7H3/b9-8-
InchiKey:	SXLJYBIAHQEULW-HJWRWDBZSA-N
Formula:	C11H22O4Si2
SMILES:	CC(=CC(=O)O[Si](C)(C)C)C(=O)O[Si](C)(C)C
Mol. weight [g/mol]:	274.46
CAS:	77220-12-3

Physical Properties

Property code	Value	Unit	Source
log10ws	1.89		Crippen Method
logp	2.689		Crippen Method
rinpol	1331.00		NIST Webbook
rinpol	1386.20		NIST Webbook
rinpol	1368.00		NIST Webbook
rinpol	1368.00		NIST Webbook
rinpol	1331.00		NIST Webbook
rinpol	1398.00		NIST Webbook
rinpol	1398.00		NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C77220123&Units=SI

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/115-513-4/Methylmaleic-acid-bis-trimethylsilyl-ester.pdf>

Generated by Cheméo on 2024-04-30 21:45:24.123217391 +0000 UTC m=+16802773.043794706.

Cheméo (<https://www.cheméo.com>) is the biggest free database of chemical and physical data for the process industry.