3-METHYLGLUTACONIC ACID diTMS (I)

Inchi:	InChI=1S/C12H24O4Si2/c1-10(8-11(13)15-17(2,3)4)9-12(14)16-18(5,6)7/h8H,9H2,1-7H3
InchiKey:	CWJVRLKZONLMHK-UHFFFAOYSA-N
Formula:	C12H24O4Si2
SMILES:	CC(=CC(=O)O[Si](C)(C)C)CC(=O)O[Si](C)(C)C
Mol. weight [g/mol]:	288.49

Physical Properties

Property code	Value	Unit	Source
log10ws	1.47		Crippen Method
logp	3.079		Crippen Method
rinpol	1450.00		NIST Webbook

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R395889&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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.chemeo.com/cid/25-450-4/3-METHYLGLUTACONIC-ACID-diTMS-I.pdf

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