

Mesaconic acid, bis(tert-butyldimethylsilyl) ester

Other names:	2-Methylfumarcic acid, TBDMS Methylmaleic acid, 2tdms derivative
Inchi:	InChI=1S/C17H34O4Si2/c1-13(15(19)21-23(10,11)17(5,6)7)12-14(18)20-22(8,9)16(2,3)4
InchiKey:	HUKRUXTVYKXRNV-OUKQBFOZSA-N
Formula:	C17H34O4Si2
SMILES:	CC(=CC(=O)O[Si](C)(C)C(C)(C)C)C(=O)O[Si](C)(C)C(C)(C)C
Mol. weight [g/mol]:	358.62

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.62		Crippen Method
logp	5.029		Crippen Method
rinpol	1823.50		NIST Webbook
rinpol	1831.00		NIST Webbook
rinpol	1831.00		NIST Webbook
rinpol	1823.50		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=U333773&Units=SI

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/117-153-2/Mesaconic-acid-bis-tert-butyldimethylsilyl-ester.pdf>

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