

Malic acid, 4-ethyl ester, 2TMS

Inchi:	InChI=1S/C12H26O5Si2/c1-8-15-11(13)9-10(16-18(2,3)4)12(14)17-19(5,6)7/h10H,8-9H2
InchiKey:	ACCAFWMWOKAAURJ-UHFFFAOYSA-N
Formula:	C12H26O5Si2
SMILES:	CCOC(=O)CC(O[Si](C)(C)C)C(=O)O[Si](C)(C)C
Mol. weight [g/mol]:	306.50

Physical Properties

Property code	Value	Unit	Source
log10ws	2.13		Crippen Method
logp	2.538		Crippen Method
rinpol	1441.70		NIST Webbook
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Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U414035&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I

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/113-537-0/Malic-acid-4-ethyl-ester-2TMS.pdf>

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