

Malic acid 1-ethyl ester, 2TMS

Inchi: InChI=1S/C12H26O5Si2/c1-8-15-12(14)10(16-18(2,3)4)9-11(13)17-19(5,6)7/h10H,8-9H2
InchiKey: LGUPUKBINNQZH-Z-UHFFFAOYSA-N
Formula: C₁₂H₂₆O₅Si₂
SMILES: CCOC(=O)C(CC(=O)O[Si](C)(C)C)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	1425.50		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=U414034&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/113-536-1/Malic-acid-1-ethyl-ester-2TMS.pdf>

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