

Mono-ethylmalonate, tert-butyldimethylsilyl ester

Other names:	Ethylmalonate, TBDMS Mono-ethyl malonate, tbdms derivative
Inchi:	InChI=1S/C11H22O4Si/c1-7-14-9(12)8-10(13)15-16(5,6)11(2,3)4/h7-8H2,1-6H3
InchiKey:	AFEMUXVHVAWNOP-UHFFFAOYSA-N
Formula:	C11H22O4Si
SMILES:	CCOC(=O)CC(=O)O[Si](C)(C)C(C)(C)C
Mol. weight [g/mol]:	246.38

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.20		Crippen Method
logp	2.488		Crippen Method
rinpola	1359.10		NIST Webbook
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Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U333871&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
rinpola:	Non-polar retention indices

Latest version available from:

<https://www.chemeo.com/cid/121-839-6/Mono-ethylmalonate-tert-butyldimethylsilyl-ester.pdf>

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