

Mono-ethylmalonate, trimethylsilyl ester

Other names:	Mono-ethyl malonate, tms derivative
Inchi:	InChI=1S/C8H16O4Si/c1-5-11-7(9)6-8(10)12-13(2,3)4/h5-6H2,1-4H3
InchiKey:	PVXMKQLVICGFSI-UHFFFAOYSA-N
Formula:	C8H16O4Si
SMILES:	CCOC(=O)CC(=O)O[Si](C)(C)C
Mol. weight [g/mol]:	204.30

Physical Properties

Property code	Value	Unit	Source
log10ws	1.05		Crippen Method
logp	1.318		Crippen Method
rinpola	1141.70		NIST Webbook
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Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U333872&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.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.cheméo.com/cid/45-748-2/Mono-ethylmalonate-trimethylsilyl-ester.pdf>

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