

Butanedioic acid, [(trimethylsilyl)oxy]-, dimethyl ester

Other names:	DL-Malic acid, O-trimethylsilyl-, dimethyl ester Dimethyl malate, tms derivative
Inchi:	InChI=1S/C9H18O5Si/c1-12-8(10)6-7(9(11)13-2)14-15(3,4)5/h7H,6H2,1-5H3
InchiKey:	MMWDFJMVASCTJS-UHFFFAOYSA-N
Formula:	C9H18O5Si
SMILES:	COC(=O)CC(O[Si](C)(C)C)C(=O)OC
Mol. weight [g/mol]:	234.32
CAS:	55590-73-3

Physical Properties

Property code	Value	Unit	Source
log10ws	1.44		Crippen Method
logp	0.943		Crippen Method
rinpol	1248.10		NIST Webbook
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Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C55590733&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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