

Ketomalonic acid, TMS

Inchi:	InChI=1S/C9H18O5Si2/c1-15(2,3)13-8(11)7(10)9(12)14-16(4,5)6/h1-6H3
InchiKey:	RVWPJPXRWFZIEK-UHFFFAOYSA-N
Formula:	C9H18O5Si2
SMILES:	C[Si](C)(C)OC(=O)C(=O)C(=O)O[Si](C)(C)C
Mol. weight [g/mol]:	262.41

Physical Properties

Property code	Value	Unit	Source
log10ws	3.30		Crippen Method
logp	1.312		Crippen Method
rinpol	1141.00		NIST Webbook

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=R401122&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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<https://www.cheméo.com/cid/19-787-8/Ketomalonic-acid-TMS.pdf>

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