

# 2-Methylacetoacetic acid, mono-TMS

**Inchi:** InChI=1S/C8H16O3Si/c1-6(7(2)9)8(10)11-12(3,4)5/h6H,1-5H3  
**InchiKey:** HDYNRULYUKFBAI-UHFFFAOYSA-N  
**Formula:** C8H16O3Si  
**SMILES:** CC(=O)C(C)C(=O)O[Si](C)(C)C  
**Mol. weight [g/mol]:** 188.30

## Physical Properties

Property code	Value	Unit	Source
log10ws	0.88		Crippen Method
logp	1.590		Crippen Method
rinpol	1087.00		NIST Webbook
rinpol	1087.00		NIST Webbook

## Sources

**Crippen Method:** <http://pubs.acs.org/doi/abs/10.1021/ci9903071>  
**Crippen Method:** [https://www.chemeo.com/doc/models/crippen\\_log10ws](https://www.chemeo.com/doc/models/crippen_log10ws)  
**NIST Webbook:** <http://webbook.nist.gov/cgi/cbook.cgi?ID=R400436&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.chemeo.com/cid/30-510-1/2-Methylacetoacetic-acid-mono-TMS.pdf>

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