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/ci990307l
Crippen Method: 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