Acetoacetic acid, MO TBDMS # 1

Inchi: InChI=1S/C11H23NO3Si/c1-9(12-14-5)8-10(13)15-16(6,7)11(2,3)4/h8H2,1-7H3
InchiKey: JLUHMJRHNTUMIH-UHFFFAOYSA-N
Formula: C11H23NO3Si
SMILES: CON=C(C)CC(=O)O[Si](C)(C)C(C)(C)C
Mol. weight [g/mol]: 245.39

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.58		Crippen Method
logp	2.947		Crippen Method
rinpol	1330.00		NIST Webbook
rinpol	1330.00		NIST Webbook

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R563894&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
rinpol: Non-polar retention indices