Acetoacetic acid, O-pentafluorobenzyloxime, TMS

Inchi: InChI=1S/C14H16F5NO3Si/c1-7(5-9(21)23-24(2,3)4)20-22-6-8-10(15)12(17)14(19)13(18

InchiKey: BTULZGHAJIMZPV-IFRROFPPSA-N

Formula: C14H16F5NO3Si

SMILES: CC(CC(=O)O[Si](C)(C)C)=NOCc1c(F)c(F)c(F)c(F)c1F

Mol. weight [g/mol]: 369.36

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.09		Crippen Method
logp	4.043		Crippen Method
rinpol	1570.00		NIST Webbook
rinpol	1592.00		NIST Webbook
rinpol	1570.00		NIST Webbook

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R315383&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