2-Ketobutyric acid pfbo-tms

Other names: Butanoic acid, 2-oxo, O-pentafluorobenzyloxime, TMS
Inchi: InChI=1S/C14H16F5NO3Si/c1-5-8(14(21)23-24(2,3)4)20-22-6-7-9(15)11(17)13(19)12(18
InchiKey: PDCPSDWZTDHPMJ-UHFFFAOYSA-N
Formula: C14H16F5NO3Si
SMILES: CCC(=NOCc1c(F)c(F)c(F)c(F)c1F)C(=O)O[Si](C)(C)C
Mol. weight [g/mol]: 369.36

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.09		Crippen Method
logp	4.043		Crippen Method
rinpol	1536.00		NIST Webbook
rinpol	1536.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U332301&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

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