2-Ketohexanoic acid pfbo-tms

Other names: Hexanoic acid, 2-oxo, O-pentafluorobenzyloxime, TMS
Inchi: InChI=1S/C16H20F5NO3Si/c1-5-6-7-10(16(23)25-26(2,3)4)22-24-8-9-11(17)13(19)15(21
InchiKey: KTEWSQYSHYTRAT-UHFFFAOYSA-N
Formula: C16H20F5NO3Si
SMILES: CCCCC(=NOCc1c(F)c(F)c(F)c(F)c1F)C(=O)O[Si](C)(C)C
Mol. weight [g/mol]: 397.41

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.93		Crippen Method
logp	4.823		Crippen Method
rinpol	1652.00		NIST Webbook
rinpol	1671.00		NIST Webbook
rinpol	1652.00		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=U332304&Units=SI

Legend

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