2-Keto-3-methylvaleric acid pfbo-tms

Other names:	2-Keto-3-methylpentanoic acid pfbo-tms
	Pentanoic acid, 3-methyl-2-oxo, O-pentafluorobenzyloxime, TMS
Inchi:	InChI=1S/C16H20F5NO3Si/c1-6-8(2)15(16(23)25-26(3,4)5)22-24-7-9-10(17)12(19)14(21
InchiKey:	VIEBVKSUXVPNCZ-UHFFFAOYSA-N
Formula:	C16H20F5NO3Si
SMILES:	CCC(C)C(=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	-3.69		Crippen Method
logp	4.679		Crippen Method
rinpol	1604.00		NIST Webbook
rinpol	1613.00		NIST Webbook
rinpol	1604.00		NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U332309&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

Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.