3-Methyl-2-ketobutyric acid pfbo-tms

Other names: Isovaleric acid, 2-oxo, O-pentafluorobenzyloxime, TMS
Inchi: InChI=1S/C15H18F5NO3Si/c1-7(2)14(15(22)24-25(3,4)5)21-23-6-8-9(16)11(18)13(20)12
InchiKey: CEGBIHRCNHPYPQ-UHFFFAOYSA-N
Formula: C15H18F5NO3Si
SMILES: CC(C)C(=NOCc1c(F)c(F)c(F)c(F)c1F)C(=O)O[Si](C)(C)C
Mol. weight [g/mol]: 383.39

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.27		Crippen Method
logp	4.289		Crippen Method
rinpol	1537.00		NIST Webbook
rinpol	1556.00		NIST Webbook
rinpol	1537.00		NIST Webbook

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U332300&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