

2-Ketoisocaproic acid pfbo-tms

Other names:	Pentanoic acid, 4-methyl-2-oxo, O-pentafluorobenzyloxime, TMS
Inchi:	InChI=1S/C16H20F5NO3Si/c1-8(2)6-10(16(23)25-26(3,4)5)22-24-7-9-11(17)13(19)15(21)20
InchiKey:	ZITNMERNWHQQFL-UHFFFAOYSA-N
Formula:	C16H20F5NO3Si
SMILES:	CC(C)CC(=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	1605.00		NIST Webbook
rinpol	1629.00		NIST Webbook
rinpol	1605.00		NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U332302&Units=SI

Legend

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

Latest version available from:

<https://www.chemeo.com/cid/117-405-2/2-Ketoisocaproic-acid-pfbo-tms.pdf>

Generated by Cheméo on 2024-05-02 17:14:06.024280703 +0000 UTC m=+16959294.944858018.

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