

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]:	397.42

Physical Properties

Property code	Value	Unit	Source
logp	4.823		Crippen Method
rinpol	1652.00		NIST Webbook
rinpol	1652.00		NIST Webbook
rinpol	1671.00		NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U332304&Units=SI

Legend

logp:	Octanol/Water partition coefficient
rinpol:	Non-polar retention indices

Latest version available from:

<https://www.chemeo.com/cid/117-409-8/2-ketohexanoic-acid-PFBO-TMS.pdf>

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