

n-Hexanal, O-[(pentafluorophenyl)methyl]oxime

Other names:	Hexanal, PFBO, # 2
Inchi:	InChI=1S/C13H14F5NO/c1-2-3-4-5-6-19-20-7-8-9(14)11(16)13(18)12(17)10(8)15/h6H,2-
InchiKey:	GPAVMFOMYSGJDM-UHFFFAOYSA-N
Formula:	C13H14F5NO
SMILES:	CCCCC=NOCc1c(F)c(F)c(F)c(F)c1F
Mol. weight [g/mol]:	295.25

Physical Properties

Property code	Value	Unit	Source
logp	4.465		Crippen Method
mcvol	190.670	ml/mol	McGowan Method
rinpol	1460.00		NIST Webbook
rinpol	1460.00		NIST Webbook
rinpol	1460.00		NIST Webbook
ripol	1765.00		NIST Webbook
ripol	1765.00		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=U288098&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume

rinpol: Non-polar retention indices

ripol: Polar retention indices

Latest version available from:

<https://www.cheméo.com/cid/117-304-4/n-Hexanal-O-pentafluorophenyl-methyl-oxime.pdf>

Generated by Cheméo on 2026-07-21 17:42:12.772292931 +0000 UTC m=+166828.614178352.

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