

2-Octanone oxime, o-[(pentafluorophenyl)methyl]-

Other names:

2-Octanone, PFBO # 2

Inchi:

InChI=1S/C15H18F5NO/c1-3-4-5-6-7-9(2)21-22-8-10-11(16)13(18)15(20)14(19)12(10)17

InchiKey:

ZKTADPFWQHMKQT-UHFFFAOYSA-N

Formula:

C15H18F5NO

SMILES:

CCCCCCC(C)=NOCc1c(F)c(F)c(F)c(F)c1F

Mol. weight [g/mol]:

323.30

Physical Properties

Property code	Value	Unit	Source
hf	-1214.09	kJ/mol	Joback Method
hvap	56.29	kJ/mol	Joback Method
log10ws	-6.60		Crippen Method
logp	5.245		Crippen Method
mcvol	218.850	ml/mol	McGowan Method
pc	1328.10	kPa	Joback Method
rinpol	1588.00		NIST Webbook
rinpol	1588.00		NIST Webbook
ripol	1833.00		NIST Webbook
ripol	1833.00		NIST Webbook
tb	689.51	K	Joback Method
tc	866.65	K	Joback Method

Sources

McGowan Method:

<http://link.springer.com/article/10.1007/BF02311772>

NIST Webbook:

<http://webbook.nist.gov/cgi/cbook.cgi?ID=U288175&Units=SI>

Crippen Method:

<http://pubs.acs.org/doi/abs/10.1021/ci9903071>

Crippen Method:

https://www.chemeo.com/doc/models/crippen_log10ws

Joback Method:

https://en.wikipedia.org/wiki/Joback_method

Legend

hf:	Enthalpy of formation at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpolar:	Non-polar retention indices
ripolar:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature

Latest version available from:

<https://www.cheméo.com/cid/117-949-9/2-Octanone-oxime-o-pentafluorophenyl-methyl.pdf>

Generated by Cheméo on 2024-04-29 03:35:23.468894542 +0000 UTC m=+16650972.389471861.

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