

# 2-Methyl-2-pentenal oxime, o-[(pentafluorophenyl)methyl]-

Other names:	(E)-2-Methyl-2-pentenal, PFBO # 2
Inchi:	InChI=1S/C13H12F5NO/c1-3-4-7(2)5-19-20-6-8-9(14)11(16)13(18)12(17)10(8)15/h4-5H,
InchiKey:	PYTSBRIQCYVWOP-YSYKFMAYSA-N
Formula:	C13H12F5NO
SMILES:	CCC=C(C)C=NOCc1c(F)c(F)c(F)c(F)c1F
Mol. weight [g/mol]:	293.23

## Physical Properties

Property code	Value	Unit	Source
hf	-1055.59	kJ/mol	Joback Method
hvap	51.80	kJ/mol	Joback Method
log10ws	-5.62		Crippen Method
logp	4.241		Crippen Method
mcvol	186.370	ml/mol	McGowan Method
pc	1600.00	kPa	Joback Method
ripol	1849.00		NIST Webbook
ripol	1849.00		NIST Webbook
tb	647.91	K	Joback Method
tc	832.12	K	Joback Method

## Sources

Joback Method:	<a href="https://en.wikipedia.org/wiki/Joback_method">https://en.wikipedia.org/wiki/Joback_method</a>
McGowan Method:	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>
NIST Webbook:	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=U288111&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U288111&amp;Units=SI</a>
Crippen Method:	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307I">http://pubs.acs.org/doi/abs/10.1021/ci990307I</a>
Crippen Method:	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>

## Legend

hf: Enthalpy of formation at standard conditions

<b>h<sub>vap</sub>:</b>	Enthalpy of vaporization at standard conditions
<b>log<sub>10</sub>w<sub>s</sub>:</b>	Log <sub>10</sub> of Water solubility in mol/l
<b>log<sub>p</sub>:</b>	Octanol/Water partition coefficient
<b>mc<sub>vol</sub>:</b>	McGowan's characteristic volume
<b>p<sub>c</sub>:</b>	Critical Pressure
<b>ri<sub>pol</sub>:</b>	Polar retention indices
<b>tb:</b>	Normal Boiling Point Temperature
<b>tc:</b>	Critical Temperature

Latest version available from:

<https://www.cheméo.com/cid/121-926-9/2-Methyl-2-pentenal-oxime-o-pentafluorophenyl-methyl.pdf>

Generated by Cheméo on 2024-05-05 06:06:15.157852888 +0000 UTC m=+17178424.078430200.

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