

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

**Other names:** 2-Methylpentanal, PFBO # 2  
**Inchi:** InChI=1S/C13H14F5NO/c1-3-4-7(2)5-19-20-6-8-9(14)11(16)13(18)12(17)10(8)15/h5,7H,  
**InchiKey:** IOULWMZNM CBDQK-UHFFFAOYSA-N  
**Formula:** C13H14F5NO  
**SMILES:** CCCC(C)C=NOCc1c(F)c(F)c(F)c(F)c1F  
**Mol. weight [g/mol]:** 295.25

## Physical Properties

Property code	Value	Unit	Source
hf	-1168.30	kJ/mol	Joback Method
hvap	51.37	kJ/mol	Joback Method
log10ws	-5.52		Crippen Method
logp	4.321		Crippen Method
mcvol	190.670	ml/mol	McGowan Method
pc	1539.08	kPa	Joback Method
rinpol	1393.00		NIST Webbook
rinpol	1393.00		NIST Webbook
tb	643.43	K	Joback Method
tc	822.07	K	Joback Method

## Sources

**Crippen Method:** <http://pubs.acs.org/doi/abs/10.1021/ci9903071>  
**Crippen Method:** [https://www.chemeo.com/doc/models/crippen\\_log10ws](https://www.chemeo.com/doc/models/crippen_log10ws)  
**Joback Method:** [https://en.wikipedia.org/wiki/Joback\\_method](https://en.wikipedia.org/wiki/Joback_method)  
**McGowan Method:** <http://link.springer.com/article/10.1007/BF02311772>  
**NIST Webbook:** <http://webbook.nist.gov/cgi/cbook.cgi?ID=U288121&Units=SI>

## 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>r<sub>inpol</sub>:</b>	Non-polar retention indices
<b>t<sub>b</sub>:</b>	Normal Boiling Point Temperature
<b>t<sub>c</sub>:</b>	Critical Temperature

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