

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

**Other names:** (E)-2-Methyl-2-butenal, PFBO # 1

**Inchi:** InChI=1S/C12H10F5NO/c1-3-6(2)4-18-19-5-7-8(13)10(15)12(17)11(16)9(7)14/h3-4H,5H2

**InchiKey:** WEZKZVIRASBEJE-BDUDBEHWSA-N

**Formula:** C12H10F5NO

**SMILES:** CC=C(C)C=NOCc1c(F)c(F)c(F)c(F)c1F

**Mol. weight [g/mol]:** 279.21

## Physical Properties

Property code	Value	Unit	Source
hf	-1034.95	kJ/mol	Joback Method
hvap	49.57	kJ/mol	Joback Method
log10ws	-5.20		Crippen Method
logp	3.851		Crippen Method
mcvol	172.280	ml/mol	McGowan Method
pc	1730.34	kPa	Joback Method
rinpol	1493.00		NIST Webbook
rinpol	1493.00		NIST Webbook
tb	625.03	K	Joback Method
tc	810.80	K	Joback Method

## Sources

**NIST Webbook:** <http://webbook.nist.gov/cgi/cbook.cgi?ID=U288144&Units=SI>

**Crippen Method:** <http://pubs.acs.org/doi/abs/10.1021/ci990307I>

**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>

## 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

Latest version available from:

<https://www.cheméo.com/cid/113-673-9/trans-2-Methyl-2-butenal-oxime-o-pentafluorophenyl-methyl.pdf>

Generated by Cheméo on 2024-04-30 12:41:45.607143766 +0000 UTC m=+16770154.527721081.

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