

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

**Other names:** (E)-2-Pentenal, PFBO # 2

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

**InchiKey:** WYODGQGHSDKODJ-GWZFUMBFA-N

**Formula:** C12H10F5NO

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

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

## Physical Properties

Property code	Value	Unit	Source
hf	-1025.16	kJ/mol	Joback Method
hvap	49.49	kJ/mol	Joback Method
log10ws	-5.20		Crippen Method
logp	3.851		Crippen Method
mcvol	172.280	ml/mol	McGowan Method
pc	1723.16	kPa	Joback Method
rinpol	1427.00		NIST Webbook
rinpol	1427.00		NIST Webbook
ripol	1825.00		NIST Webbook
ripol	1825.00		NIST Webbook
tb	625.15	K	Joback Method
tc	808.30	K	Joback Method

## Sources

**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=U288148&Units=SI>

**Crippen Method:** <http://pubs.acs.org/doi/abs/10.1021/ci990307l>

**Crippen Method:** [https://www.chemeo.com/doc/models/crippen\\_log10ws](https://www.chemeo.com/doc/models/crippen_log10ws)

# Legend

<b>hf:</b>	Enthalpy of formation at standard conditions
<b>h<sub>vap</sub>:</b>	Enthalpy of vaporization at standard conditions
<b>log<sub>10</sub>ws:</b>	Log <sub>10</sub> of Water solubility in mol/l
<b>log<sub>p</sub>:</b>	Octanol/Water partition coefficient
<b>mcvol:</b>	McGowan's characteristic volume
<b>pc:</b>	Critical Pressure
<b>rinpol:</b>	Non-polar retention indices
<b>ripol:</b>	Polar retention indices
<b>tb:</b>	Normal Boiling Point Temperature
<b>tc:</b>	Critical Temperature

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