

# Pentanal O-pentafluorophenylmethyl-oxime

<b>Other names:</b>	Pentanal O-2,3,4,5,6-PFBHA-oxime Pentanal, PFBO, # 2
<b>Inchi:</b>	InChI=1S/C12H12F5NO/c1-2-3-4-5-18-19-6-7-8(13)10(15)12(17)11(16)9(7)14/h5H,2-4,6
<b>InchiKey:</b>	CQVUQQBKUBLHIZ-UHFFFAOYSA-N
<b>Formula:</b>	C12H12F5NO
<b>SMILES:</b>	CCCCC=NOCc1c(F)c(F)c(F)c(F)c1F
<b>Mol. weight [g/mol]:</b>	281.22
<b>CAS:</b>	932710-56-0

## Physical Properties

Property code	Value	Unit	Source
hf	-1142.38	kJ/mol	Joback Method
hvap	49.53	kJ/mol	Joback Method
log10ws	-5.34		Crippen Method
logp	4.075		Crippen Method
mcvol	176.580	ml/mol	McGowan Method
pc	1651.11	kPa	Joback Method
rinpol	1366.00		NIST Webbook
rinpol	1369.00		NIST Webbook
rinpol	1369.00		NIST Webbook
ripol	1675.00		NIST Webbook
tb	620.99	K	Joback Method
tc	797.91	K	Joback Method

## Sources

<b>Joback Method:</b>	<a href="https://en.wikipedia.org/wiki/Joback_method">https://en.wikipedia.org/wiki/Joback_method</a>
<b>McGowan Method:</b>	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C932710560&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C932710560&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307I">http://pubs.acs.org/doi/abs/10.1021/ci990307I</a>
<b>Crippen Method:</b>	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>

# 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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