

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

Other names:

2-Butanone, PFBO # 2

Inchi:

InChI=1S/C11H10F5NO/c1-3-5(2)17-18-4-6-7(12)9(14)11(16)10(15)8(6)13/h3-4H2,1-2H1

InchiKey:

LNDQFOSWZJYEIC-UHFFFAOYSA-N

Formula:

C11H10F5NO

SMILES:

CCC(C)=NOCc1c(F)c(F)c(F)c(F)c1F

Mol. weight [g/mol]:

267.20

## Physical Properties

Property code	Value	Unit	Source
hf	-1131.53	kJ/mol	Joback Method
hvap	47.39	kJ/mol	Joback Method
log10ws	-4.93		Crippen Method
logp	3.685		Crippen Method
mcvol	162.490	ml/mol	McGowan Method
pc	1795.46	kPa	Joback Method
ripol	1521.00		NIST Webbook
ripol	1521.00		NIST Webbook
tb	597.99	K	Joback Method
tc	778.76	K	Joback Method

## Sources

NIST Webbook:

<http://webbook.nist.gov/cgi/cbook.cgi?ID=U288170&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>ri<sub>pol</sub>:</b>	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/121-472-3/2-Butanone-oxime-o-pentafluorophenyl-methyl.pdf>

Generated by Cheméo on 2024-04-28 00:49:40.353842792 +0000 UTC m=+16554629.274420107.

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