# n-Heptanal, o-[(pentafluorophenyl)methyl]oxime

**Other names:** Heptanal, PFBO # 2
**Inchi:** InChI=1S/C14H16F5NO/c1-2-3-4-5-6-7-20-21-8-9-10(15)12(17)14(19)13(18)11(9)16/h7H
**InchiKey:** OZZBQOMRSSEYJF-UHFFFAOYSA-N
**Formula:** C14H16F5NO
**SMILES:** CCCCCCC=NOCc1c(F)c(F)c(F)c(F)c1F
**Mol. weight [g/mol]:** 309.27

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| hf | -1183.66 | kJ/mol | Joback Method |
| hvap | 53.98 | kJ/mol | Joback Method |
| log10ws | -6.18 | | Crippen Method |
| logp | 4.855 | | Crippen Method |
| mcvol | 204.760 | ml/mol | McGowan Method |
| pc | 1420.78 | kPa | Joback Method |
| rinpol | 1558.00 | | NIST Webbook |
| rinpol | 1558.00 | | NIST Webbook |
| ripol | 1861.00 | | NIST Webbook |
| tb | 666.75 | K | Joback Method |
| tc | 842.19 | K | Joback Method |

## Sources

**Crippen Method:** http://pubs.acs.org/doi/abs/10.1021/ci990307l
**Crippen Method:** https://www.chemeo.com/doc/models/crippen_log10ws
**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=U288096&Units=SI

## Legend

| | |
|---|---|
| **hf:** | Enthalpy of formation at standard conditions |
| **hvap:** | Enthalpy of vaporization at standard conditions |
| **log10ws:** | Log10 of Water solubility in mol/l |
| **logp:** | Octanol/Water partition coefficient |
| **mcvol:** | McGowan's characteristic volume |
| **pc:** | Critical Pressure |
| **rinpol:** | Non-polar retention indices |
| **ripol:** | Polar retention indices |
| **tb:** | Normal Boiling Point Temperature |
| **tc:** | Critical Temperature |