

# Heptanal, PFBO # 1

**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:** CCCCCC=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
rinsol	1551.00		NIST Webbook
ripol	1852.00		NIST Webbook
ripol	1852.00		NIST Webbook
tb	666.75	K	Joback Method
tc	842.19	K	Joback Method

## Sources

**NIST Webbook:** <http://webbook.nist.gov/cgi/cbook.cgi?ID=R575763&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)  
**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>hvap:</b>	Enthalpy of vaporization at standard conditions
<b>log10ws:</b>	Log10 of Water solubility in mol/l
<b>logp:</b>	Octanol/Water partition coefficient
<b>mccvol:</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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