

# (E,E)-2,4-Hexadienal, PFBO # 1

**Inchi:** InChI=1S/C13H10F5NO/c1-2-3-4-5-6-19-20-7-8-9(14)11(16)13(18)12(17)10(8)15/h2-6H,  
**InchiKey:** LLOGYFAPZSCQBM-XKLQSORGSA-N  
**Formula:** C13H10F5NO  
**SMILES:** CC=CC=CC=NOCc1c(F)c(F)c(F)c(F)c1F  
**Mol. weight [g/mol]:** 291.22

## Physical Properties

Property code	Value	Unit	Source
hf	-928.58	kJ/mol	Joback Method
hvap	51.67	kJ/mol	Joback Method
log10ws	-5.47		Crippen Method
logp	4.017		Crippen Method
mcvol	182.070	ml/mol	McGowan Method
pc	1661.90	kPa	Joback Method
rinpol	1591.00		NIST Webbook
ripol	2079.00		NIST Webbook
tb	652.19	K	Joback Method
tc	840.19	K	Joback Method

## Sources

**McGowan Method:** <http://link.springer.com/article/10.1007/BF02311772>  
**NIST Webbook:** <http://webbook.nist.gov/cgi/cbook.cgi?ID=R575649&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)

## Legend

**hf:** Enthalpy of formation at standard conditions  
**hvap:** Enthalpy of vaporization at standard conditions

<b>log10ws:</b>	Log10 of Water solubility in mol/l
<b>logp:</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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