

# (E)-2-Heptenal, PFBO # 1

**Inchi:** InChI=1S/C14H14F5NO/c1-2-3-4-5-6-7-20-21-8-9-10(15)12(17)14(19)13(18)11(9)16/h5-  
**InchiKey:** PEYJSQOBEFLESI-HXIWAJJLSA-N  
**Formula:** C14H14F5NO  
**SMILES:** CCCCC=CC=NOCc1c(F)c(F)c(F)c(F)c1F  
**Mol. weight [g/mol]:** 307.26

## Physical Properties

Property code	Value	Unit	Source
hf	-1066.44	kJ/mol	Joback Method
hvap	53.94	kJ/mol	Joback Method
log10ws	-6.03		Crippen Method
logp	4.631		Crippen Method
mcvol	200.460	ml/mol	McGowan Method
pc	1478.15	kPa	Joback Method
rinpol	1626.00		NIST Webbook
rinpol	1626.00		NIST Webbook
ripol	2009.00		NIST Webbook
ripol	2009.00		NIST Webbook
tb	670.91	K	Joback Method
tc	851.69	K	Joback Method

## Sources

**NIST Webbook:** <http://webbook.nist.gov/cgi/cbook.cgi?ID=R575461&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

<b>hf:</b>	Enthalpy of formation at standard conditions
<b>hvac:</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>mcvol:</b>	McGowan's characteristic volume
<b>pc:</b>	Critical Pressure
<b>rinpolar:</b>	Non-polar retention indices
<b>ripolar:</b>	Polar retention indices
<b>tb:</b>	Normal Boiling Point Temperature
<b>tc:</b>	Critical Temperature

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