

# Acetophenone, PFBO # 1

**Inchi:** InChI=1S/C15H10F5NO/c1-8(9-5-3-2-4-6-9)21-22-7-10-11(16)13(18)15(20)14(19)12(10)  
**InchiKey:** MICGAUDRWWJXQO-UHFFFAOYSA-N  
**Formula:** C15H10F5NO  
**SMILES:** CC(=NOc1c(F)c(F)c(F)c1F)c1ccccc1  
**Mol. weight [g/mol]:** 315.24

## Physical Properties

Property code	Value	Unit	Source
hf	-977.56	kJ/mol	Joback Method
hvap	58.57	kJ/mol	Joback Method
log10ws	-5.80		Crippen Method
logp	4.323		Crippen Method
mcvol	195.090	ml/mol	McGowan Method
pc	1717.45	kPa	Joback Method
rinpol	1646.00		NIST Webbook
ripol	2171.00		NIST Webbook
tb	716.19	K	Joback Method
tc	921.45	K	Joback Method

## Sources

**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>  
**NIST Webbook:** <http://webbook.nist.gov/cgi/cbook.cgi?ID=R575223&Units=SI>  
**Crippen Method:** <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

## 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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