

# Propanal, PFBO # 1

**Inchi:** InChI=1S/C10H8F5NO/c1-2-3-16-17-4-5-6(11)8(13)10(15)9(14)7(5)12/h3H,2,4H2,1H3/b  
**InchiKey:** BOPZGAUHLLBMFA-HQYXKAPLSA-N  
**Formula:** C10H8F5NO  
**SMILES:** CCC=NOCc1c(F)c(F)c(F)c(F)c1F  
**Mol. weight [g/mol]:** 253.17

## Physical Properties

Property code	Value	Unit	Source
hf	-1101.10	kJ/mol	Joback Method
hvap	45.08	kJ/mol	Joback Method
log10ws	-4.51		Crippen Method
logp	3.295		Crippen Method
mcvol	148.400	ml/mol	McGowan Method
pc	1942.37	kPa	Joback Method
rinpol	1187.00		NIST Webbook
rinpol	1187.00		NIST Webbook
ripol	1502.00		NIST Webbook
ripol	1502.00		NIST Webbook
tb	575.23	K	Joback Method
tc	754.89	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=R575867&Units=SI>  
**Crippen Method:** <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

## 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>rinpola:</b>	Non-polar retention indices
<b>ripola:</b>	Polar retention indices
<b>tb:</b>	Normal Boiling Point Temperature
<b>tc:</b>	Critical Temperature

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