

# 2-Pentanone, 4-methyl-4-methylthio, PFBO # 1

**Inchi:** InChI=1S/C14H16F5NOS/c1-7(5-14(2,3)22-4)20-21-6-8-9(15)11(17)13(19)12(18)10(8)16  
**InchiKey:** NFLXDNDKDYWMBT-UHFFFAOYSA-N  
**Formula:** C14H16F5NOS  
**SMILES:** CSC(C)(C)CC(C)=NOCc1c(F)c(F)c(F)c(F)c1F  
**Mol. weight [g/mol]:** 341.34

## Physical Properties

Property code	Value	Unit	Source
hf	-1160.33	kJ/mol	Joback Method
hvap	59.58	kJ/mol	Joback Method
log10ws	-6.18		Crippen Method
logp	4.806		Crippen Method
mcvol	221.110	ml/mol	McGowan Method
pc	1465.73	kPa	Joback Method
rinpola	1969.00		NIST Webbook
rinpola	1969.00		NIST Webbook
ripola	2098.00		NIST Webbook
tb	732.18	K	Joback Method
tc	931.06	K	Joback Method

## Sources

**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=R574839&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)

## Legend

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

<b>h<sub>vap</sub>:</b>	Enthalpy of vaporization at standard conditions
<b>log<sub>10</sub>w<sub>s</sub>:</b>	Log10 of Water solubility in mol/l
<b>log<sub>p</sub>:</b>	Octanol/Water partition coefficient
<b>m<sub>cvol</sub>:</b>	McGowan's characteristic volume
<b>p<sub>c</sub>:</b>	Critical Pressure
<b>r<sub>inpol</sub>:</b>	Non-polar retention indices
<b>r<sub>ipol</sub>:</b>	Polar retention indices
<b>t<sub>b</sub>:</b>	Normal Boiling Point Temperature
<b>t<sub>c</sub>:</b>	Critical Temperature

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