

# Bicyclo[2.1.0]pentane, 2,2,3,3-tetrafluoro-5-methyl-, (1 «alpha», 4 «alpha», 5 «beta»)-

InChI: InChI=1S/C6H6F4/c1-2-3-4(2)6(9,10)5(3,7)8/h2-4H,1H3/t2-,3+,4-  
InChIKey: YBDXR0WBS0GEOB-YFUJLLDVSA-N

Formula: C6H6F4  
SMILES: CC1C2C1C(F)(F)C2(F)F  
Mol. weight [g/mol]: 154.11  
CAS: 87144-71-6

## Physical Properties

Property code	Value	Unit	Source
gf	-680.11	kJ/mol	Joback Method
hf	-830.39	kJ/mol	Joback Method
hfus	12.60	kJ/mol	Joback Method
hvap	22.11	kJ/mol	Joback Method
log10ws	-2.03		Crippen Method
logp	2.153		Crippen Method
mcvol	80.760	ml/mol	McGowan Method
pc	3272.78	kPa	Joback Method
tb	329.44	K	Joback Method
tc	489.39	K	Joback Method
tf	234.22	K	Joback Method
vc	0.358	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	156.63	J/molxK	329.44	Joback Method
cpg	170.61	J/molxK	356.10	Joback Method
cpg	183.34	J/molxK	382.76	Joback Method
cpg	194.92	J/molxK	409.41	Joback Method
cpg	205.45	J/molxK	436.07	Joback Method
cpg	215.01	J/molxK	462.73	Joback Method
cpg	223.70	J/molxK	489.39	Joback Method

# Sources

<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307l">http://pubs.acs.org/doi/abs/10.1021/ci990307l</a>
<b>Crippen Method:</b>	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>
<b>Joback Method:</b>	<a href="https://en.wikipedia.org/wiki/Joback_method">https://en.wikipedia.org/wiki/Joback_method</a>
<b>McGowan Method:</b>	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C87144716&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C87144716&amp;Units=SI</a>

# Legend

<b>cpg:</b>	Ideal gas heat capacity
<b>gf:</b>	Standard Gibbs free energy of formation
<b>hf:</b>	Enthalpy of formation at standard conditions
<b>hfus:</b>	Enthalpy of fusion at standard conditions
<b>h vap:</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>m cvol:</b>	McGowan's characteristic volume
<b>pc:</b>	Critical Pressure
<b>tb:</b>	Normal Boiling Point Temperature
<b>tc:</b>	Critical Temperature
<b>tf:</b>	Normal melting (fusion) point
<b>vc:</b>	Critical Volume

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