

# 2-Fluoro-5-(trifluoromethyl)propiophenone

<b>Inchi:</b>	InChI=1S/C10H8F4O/c1-2-9(15)7-5-6(10(12,13)14)3-4-8(7)11/h3-5H,2H2,1H3
<b>InchiKey:</b>	SCKAMDGXXQFMFY-UHFFFAOYSA-N
<b>Formula:</b>	C10H8F4O
<b>SMILES:</b>	CCC(=O)c1cc(C(F)(F)F)ccc1F
<b>Mol. weight [g/mol]:</b>	220.16
<b>CAS:</b>	207974-18-3

## Physical Properties

Property code	Value	Unit	Source
gf	-778.85	kJ/mol	Joback Method
hf	-941.91	kJ/mol	Joback Method
hfus	21.42	kJ/mol	Joback Method
hvap	43.64	kJ/mol	Joback Method
log10ws	-3.99		Crippen Method
logp	3.437		Crippen Method
mcvol	136.650	ml/mol	McGowan Method
pc	2563.69	kPa	Joback Method
tb	512.56	K	Joback Method
tc	701.16	K	Joback Method
tf	308.63	K	Joback Method
vc	0.554	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	313.15	J/molxK	512.56	Joback Method
cpg	324.79	J/molxK	543.99	Joback Method
cpg	335.71	J/molxK	575.43	Joback Method
cpg	345.96	J/molxK	606.86	Joback Method
cpg	355.55	J/molxK	638.29	Joback Method
cpg	364.53	J/molxK	669.73	Joback Method
cpg	372.92	J/molxK	701.16	Joback Method

# Sources

<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</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=C207974183&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C207974183&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>hvap:</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>mccvol:</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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