

# Acetophenone, 3'-fluoro-4'-methoxy-

<b>Other names:</b>	3'-Fluoro-4'-methoxyacetophenone 3-Fluoro-4-methoxyacetophenone Ethanone, 1-(3-fluoro-4-methoxyphenyl)- 1-(3-fluoro-4-methoxyphenyl)ethan-1-one
<b>Inchi:</b>	InChI=1S/C9H9FO2/c1-6(11)7-3-4-9(12-2)8(10)5-7/h3-5H,1-2H3
<b>InchiKey:</b>	LQASUDVYVOFKNK-UHFFFAOYSA-N
<b>Formula:</b>	C9H9FO2
<b>SMILES:</b>	COc1ccc(C(C)=O)cc1F
<b>Mol. weight [g/mol]:</b>	168.16
<b>CAS:</b>	455-91-4

## Physical Properties

Property code	Value	Unit	Source
gf	-310.68	kJ/mol	Joback Method
hf	-456.41	kJ/mol	Joback Method
hfus	18.20	kJ/mol	Joback Method
hvap	47.57	kJ/mol	Joback Method
log10ws	-2.58		Crippen Method
logp	2.037		Crippen Method
mcvol	123.120	ml/mol	McGowan Method
pc	3156.17	kPa	Joback Method
tb	517.52	K	Joback Method
tc	724.99	K	Joback Method
tf	315.40	K	Joback Method
vc	0.473	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	264.31	J/molxK	517.52	Joback Method
cpg	275.58	J/molxK	552.10	Joback Method
cpg	286.31	J/molxK	586.68	Joback Method
cpg	296.50	J/molxK	621.26	Joback Method
cpg	306.15	J/molxK	655.83	Joback Method

cpg	315.26	J/mol×K	690.41	Joback Method
cpg	323.85	J/mol×K	724.99	Joback Method

## Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	420.70	K	2.70	NIST Webbook

## Sources

<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=C455914&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C455914&amp;Units=SI</a>
<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>

## 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>mcvol:</b>	McGowan's characteristic volume
<b>pc:</b>	Critical Pressure
<b>tb:</b>	Normal Boiling Point Temperature
<b>tbrp:</b>	Boiling point at reduced pressure
<b>tc:</b>	Critical Temperature
<b>tf:</b>	Normal melting (fusion) point
<b>vc:</b>	Critical Volume

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