

# Formic acid, (3-methoxy-4-nitrophenyl)methyl ester

Inchi:	InChI=1S/C9H9NO5/c1-14-9-4-7(5-15-6-11)2-3-8(9)10(12)13/h2-4,6H,5H2,1H3
InchiKey:	WFSUXNOPTQWGRR-UHFFFAOYSA-N
Formula:	C9H9NO5
SMILES:	<chem>COc1cc(COC=O)ccc1[N+](=O)[O-]</chem>
Mol. weight [g/mol]:	211.17

## Physical Properties

Property code	Value	Unit	Source
gf	-155.92	kJ/mol	Joback Method
hf	-376.28	kJ/mol	Joback Method
hfus	28.36	kJ/mol	Joback Method
hvap	67.36	kJ/mol	Joback Method
log10ws	-2.40		Crippen Method
logp	1.276		Crippen Method
mvol	144.640	ml/mol	McGowan Method
pc	3345.11	kPa	Joback Method
rinpol	1795.00		NIST Webbook
tb	687.30	K	Joback Method
tc	921.78	K	Joback Method
tf	472.72	K	Joback Method
vc	0.567	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	368.54	J/mol×K	687.30	Joback Method
cpg	379.40	J/mol×K	726.38	Joback Method
cpg	389.47	J/mol×K	765.46	Joback Method
cpg	398.75	J/mol×K	804.54	Joback Method
cpg	407.24	J/mol×K	843.62	Joback Method
cpg	414.92	J/mol×K	882.70	Joback Method
cpg	421.78	J/mol×K	921.78	Joback Method

# Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=U368929&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U368929&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>
<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>

# 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>rinpola:</b>	Non-polar retention indices
<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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