

# Benzoyl chloride, 3-methoxy-

<b>Other names:</b>	m-Anisoyl chloride Benzoyl chloride, m-methoxy- m-Methoxybenzoyl chloride 3-Methoxybenzoyl chloride
<b>Inchi:</b>	InChI=1S/C8H7ClO2/c1-11-7-4-2-3-6(5-7)8(9)10/h2-5H,1H3
<b>InchiKey:</b>	RUQUIASLAXJZIE-UHFFFAOYSA-N
<b>Formula:</b>	C8H7ClO2
<b>SMILES:</b>	COc1cccc(C(=O)Cl)c1
<b>Mol. weight [g/mol]:</b>	170.59
<b>CAS:</b>	1711-05-3

## Physical Properties

Property code	Value	Unit	Source
gf	-126.59	kJ/mol	Joback Method
hf	-243.93	kJ/mol	Joback Method
hfus	17.11	kJ/mol	Joback Method
hvap	49.88	kJ/mol	Joback Method
log10ws	-2.48		Crippen Method
logp	2.074		Crippen Method
mcvol	119.500	ml/mol	McGowan Method
pc	3624.61	kPa	Joback Method
tb	527.82	K	Joback Method
tc	753.98	K	Joback Method
tf	320.94	K	Joback Method
vc	0.449	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	237.52	J/molxK	527.82	Joback Method
cpg	247.94	J/molxK	565.51	Joback Method
cpg	257.76	J/molxK	603.21	Joback Method
cpg	266.97	J/molxK	640.90	Joback Method
cpg	275.58	J/molxK	678.59	Joback Method

cpg	283.61	J/molxK	716.28	Joback Method
cpg	291.07	J/molxK	753.98	Joback Method
dvisc	0.0017026	Paxs	320.94	Joback Method
dvisc	0.0010543	Paxs	355.42	Joback Method
dvisc	0.0007106	Paxs	389.90	Joback Method
dvisc	0.0005107	Paxs	424.38	Joback Method
dvisc	0.0003857	Paxs	458.86	Joback Method
dvisc	0.0003030	Paxs	493.34	Joback Method
dvisc	0.0002456	Paxs	527.82	Joback Method

## Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	397.20	K	2.00	NIST Webbook

## Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C1711053&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C1711053&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>dvisc:</b>	Dynamic viscosity
<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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