

# Carbamic chloride, methylphenyl-

<b>Other names:</b>	N-Methyl-N-phenylcarbamoyl chloride Carbamoyl chloride, methylphenyl- Carbaniloyl chloride, N-methyl- Methylphenylcarbamoyl chloride
<b>Inchi:</b>	InChI=1S/C8H8ClNO/c1-10(8(9)11)7-5-3-2-4-6-7/h2-6H,1H3
<b>InchiKey:</b>	CPGWSLFYXMRNDV-UHFFFAOYSA-N
<b>Formula:</b>	C8H8ClNO
<b>SMILES:</b>	CN(C(=O)Cl)c1ccccc1
<b>Mol. weight [g/mol]:</b>	169.61
<b>CAS:</b>	4285-42-1

## Physical Properties

Property code	Value	Unit	Source
gf	98.82	kJ/mol	Joback Method
hf	-32.71	kJ/mol	Joback Method
hfus	19.33	kJ/mol	Joback Method
hvap	48.85	kJ/mol	Joback Method
log10ws	-2.29		Crippen Method
logp	2.482		Crippen Method
mcvol	123.610	ml/mol	McGowan Method
pc	3759.17	kPa	Joback Method
tb	553.20	K	NIST Webbook
tc	736.96	K	Joback Method
tf	318.66	K	Joback Method
vc	0.449	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	248.54	J/molxK	512.86	Joback Method
cpg	260.50	J/molxK	550.21	Joback Method
cpg	271.58	J/molxK	587.56	Joback Method
cpg	281.82	J/molxK	624.91	Joback Method
cpg	291.29	J/molxK	662.26	Joback Method

cpg	300.01	J/mol×K	699.61	Joback Method
cpg	308.04	J/mol×K	736.96	Joback Method

## Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C4285421&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C4285421&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>hvac:</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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