

# o-Nitrobenzoyl chloride

<b>Other names:</b>	2-Nitrobenzoyl chloride Benzoyl chloride, 2-nitro- Benzoyl chloride, o-nitro-
<b>Inchi:</b>	InChI=1S/C7H4ClNO3/c8-7(10)5-3-1-2-4-6(5)9(11)12/h1-4H
<b>InchiKey:</b>	BWWHTIHDQBHTHP-UHFFFAOYSA-N
<b>Formula:</b>	C7H4ClNO3
<b>SMILES:</b>	O=C(Cl)c1cccc1[N+](=O)[O-]
<b>Mol. weight [g/mol]:</b>	185.56
<b>CAS:</b>	610-14-0

## Physical Properties

Property code	Value	Unit	Source
gf	5.54	kJ/mol	Joback Method
hf	-101.83	kJ/mol	Joback Method
hfus	24.70	kJ/mol	Joback Method
hvap	61.84	kJ/mol	Joback Method
log10ws	-3.01		Crippen Method
logp	1.974		Crippen Method
mcvol	116.960	ml/mol	McGowan Method
pc	4238.55	kPa	Joback Method
tb	634.36	K	Joback Method
tc	895.19	K	Joback Method
tf	431.05	K	Joback Method
vc	0.457	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	250.84	J/molxK	634.36	Joback Method
cpg	259.60	J/molxK	677.83	Joback Method
cpg	267.55	J/molxK	721.30	Joback Method
cpg	274.74	J/molxK	764.78	Joback Method
cpg	281.22	J/molxK	808.25	Joback Method
cpg	287.03	J/molxK	851.72	Joback Method

## Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	421.70	K	1.00	NIST Webbook

## Sources

<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=C610140&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C610140&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>

## 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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