

# Phenol, 2-nitro-3,4,6-trichloro-

<b>Other names:</b>	2-Nitro-3,4,6-trichlorophenol 3,4,6-Trichloro-2-nitrophenol Phenol, 3,4,6-trichloro-2-nitro-
<b>Inchi:</b>	InChI=1S/C6H2Cl3NO3/c7-2-1-3(8)6(11)5(4(2)9)10(12)13/h1,11H
<b>InchiKey:</b>	XWLBYVXDCGYXGY-UHFFFAOYSA-N
<b>Formula:</b>	C6H2Cl3NO3
<b>SMILES:</b>	O=[N+]([O-])c1c(O)c(Cl)cc(Cl)c1Cl
<b>Mol. weight [g/mol]:</b>	242.44
<b>CAS:</b>	82-62-2

## Physical Properties

Property code	Value	Unit	Source
gf	-71.70	kJ/mol	Joback Method
hf	-200.34	kJ/mol	Joback Method
hfus	33.90	kJ/mol	Joback Method
hvap	75.97	kJ/mol	Joback Method
log10ws	-3.73		Crippen Method
logp	3.261		Crippen Method
mcvol	131.650	ml/mol	McGowan Method
pc	4704.19	kPa	Joback Method
tb	723.05	K	Joback Method
tc	997.82	K	Joback Method
tf	365.00 ± 2.00	K	NIST Webbook
vc	0.459	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	264.61	J/mol×K	723.05	Joback Method
cpg	270.14	J/mol×K	768.84	Joback Method
cpg	275.31	J/mol×K	814.64	Joback Method
cpg	280.21	J/mol×K	860.43	Joback Method
cpg	284.96	J/mol×K	906.23	Joback Method
cpg	289.68	J/mol×K	952.02	Joback Method

## Sources

<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=C82622&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C82622&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307l">http://pubs.acs.org/doi/abs/10.1021/ci990307l</a>
<b>Crippen Method:</b>	<a href="https://www.cheméo.com/doc/models/crippen_log10ws">https://www.cheméo.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>

## 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>tc:</b>	Critical Temperature
<b>tf:</b>	Normal melting (fusion) point
<b>vc:</b>	Critical Volume

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