

# Anthraquinone, 1-chloro-5-nitro

<b>Other names:</b>	1-Chloro-5-nitroanthraquinone
<b>Inchi:</b>	InChI=1S/C14H6ClNO4/c15-9-5-1-3-7-11(9)13(17)8-4-2-6-10(16(19)20)12(8)14(7)18/h1-
<b>InchiKey:</b>	VOZLLWQPJJSWPR-UHFFFAOYSA-N
<b>Formula:</b>	C14H6ClNO4
<b>SMILES:</b>	O=C1c2cccc([N+](=O)[O-])c2C(=O)c2cccc(Cl)c21
<b>Mol. weight [g/mol]:</b>	287.65
<b>CAS:</b>	129-40-8

## Physical Properties

Property code	Value	Unit	Source
gf	112.30	kJ/mol	Joback Method
hf	-107.71	kJ/mol	Joback Method
hfus	32.28	kJ/mol	Joback Method
hvap	83.48	kJ/mol	Joback Method
log10ws	-4.97		Crippen Method
logp	3.024		Crippen Method
mcvol	182.540	ml/mol	McGowan Method
pc	3166.83	kPa	Joback Method
tb	925.05	K	Joback Method
tc	1215.77	K	Joback Method
tf	686.13	K	Joback Method
vc	0.715	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	502.51	J/molxK	925.05	Joback Method
cpg	511.87	J/molxK	973.50	Joback Method
cpg	519.97	J/molxK	1021.96	Joback Method
cpg	526.85	J/molxK	1070.41	Joback Method
cpg	532.55	J/molxK	1118.87	Joback Method
cpg	537.13	J/molxK	1167.32	Joback Method
cpg	540.63	J/molxK	1215.77	Joback Method

# Sources

<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>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C129408&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C129408&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307I">http://pubs.acs.org/doi/abs/10.1021/ci990307I</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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