

# 4-Nitrobenzoic acid, 4-chlorophenyl ester

<b>Inchi:</b>	InChI=1S/C13H8ClNO4/c14-10-3-7-12(8-4-10)19-13(16)9-1-5-11(6-2-9)15(17)18/h1-8H
<b>InchiKey:</b>	FYLVXSFYEBNIKC-UHFFFAOYSA-N
<b>Formula:</b>	C13H8ClNO4
<b>SMILES:</b>	O=C(Oc1ccc(Cl)cc1)c1ccc([N+](=O)[O-])cc1
<b>Mol. weight [g/mol]:</b>	277.66

## Physical Properties

Property code	Value	Unit	Source
gf	53.84	kJ/mol	Joback Method
hf	-132.83	kJ/mol	Joback Method
hfus	35.07	kJ/mol	Joback Method
hvap	80.54	kJ/mol	Joback Method
log10ws	-4.89		Crippen Method
logp	3.467		Crippen Method
mvol	183.610	ml/mol	McGowan Method
pc	3042.32	kPa	Joback Method
rinpol	2225.00		NIST Webbook
rinpol	2225.00		NIST Webbook
tb	825.72	K	Joback Method
tc	1095.18	K	Joback Method
tf	559.84	K	Joback Method
vc	0.703	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	475.52	J/mol×K	825.72	Joback Method
cpg	485.78	J/mol×K	870.63	Joback Method
cpg	494.85	J/mol×K	915.54	Joback Method
cpg	502.79	J/mol×K	960.45	Joback Method
cpg	509.67	J/mol×K	1005.36	Joback Method
cpg	515.53	J/mol×K	1050.27	Joback Method
cpg	520.45	J/mol×K	1095.18	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=U308010&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U308010&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>hvp:</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>rlnol:</b>	Non-polar retention indices
<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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