

# 4-Nitrophenyl chloroacetate

<b>Other names:</b>	Chloroacetic acid, 4-nitrophenyl ester
<b>Inchi:</b>	InChI=1S/C8H6ClNO4/c9-5-8(11)14-7-3-1-6(2-4-7)10(12)13/h1-4H,5H2
<b>InchiKey:</b>	DYFFUJNIXCDLOR-UHFFFAOYSA-N
<b>Formula:</b>	C8H6ClNO4
<b>SMILES:</b>	O=C(CCl)Oc1ccc([N+](=O)[O-])cc1
<b>Mol. weight [g/mol]:</b>	215.59
<b>CAS:</b>	79328-69-1

## Physical Properties

Property code	Value	Unit	Source
gf	-91.04	kJ/mol	Joback Method
hf	-254.69	kJ/mol	Joback Method
hfus	28.47	kJ/mol	Joback Method
hvap	66.47	kJ/mol	Joback Method
log10ws	-2.59		Crippen Method
logp	1.739		Crippen Method
mcvol	136.920	ml/mol	McGowan Method
pc	3677.55	kPa	Joback Method
rinpol	1667.00		NIST Webbook
rinpol	1667.00		NIST Webbook
tb	679.66	K	Joback Method
tc	929.97	K	Joback Method
tf	464.55	K	Joback Method
vc	0.530	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	318.83	J/molxK	679.66	Joback Method
cpg	328.44	J/molxK	721.38	Joback Method
cpg	337.23	J/molxK	763.10	Joback Method
cpg	345.21	J/molxK	804.82	Joback Method
cpg	352.41	J/molxK	846.53	Joback Method
cpg	358.85	J/molxK	888.25	Joback Method

## Sources

<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>
<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=C79328691&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C79328691&amp;Units=SI</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>rinpol:</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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