

# 2,4-Dichloro-«omega»-nitrostyrene

<b>Inchi:</b>	InChI=1S/C8H5Cl2NO2/c9-7-2-1-6(8(10)5-7)3-4-11(12)13/h1-5H/b4-3+
<b>InchiKey:</b>	LIWIJBBAMBDXME-ONEGZZNKSA-N
<b>Formula:</b>	C8H5Cl2NO2
<b>SMILES:</b>	O=[N+]([O-])C=Cc1ccc(Cl)cc1Cl
<b>Mol. weight [g/mol]:</b>	218.04
<b>CAS:</b>	34209-97-7

## Physical Properties

Property code	Value	Unit	Source
gf	201.54	kJ/mol	Joback Method
hf	80.12	kJ/mol	Joback Method
hfus	29.70	kJ/mol	Joback Method
hvap	62.32	kJ/mol	Joback Method
log10ws	-4.24		Crippen Method
logp	3.241		Crippen Method
mcvol	137.420	ml/mol	McGowan Method
pc	3480.65	kPa	Joback Method
tb	649.94	K	Joback Method
tc	913.47	K	Joback Method
tf	429.75	K	Joback Method
vc	0.535	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	285.32	J/molxK	649.94	Joback Method
cpg	294.45	J/molxK	693.86	Joback Method
cpg	302.77	J/molxK	737.78	Joback Method
cpg	310.35	J/molxK	781.71	Joback Method
cpg	317.26	J/molxK	825.63	Joback Method
cpg	323.59	J/molxK	869.55	Joback Method
cpg	329.41	J/molxK	913.47	Joback Method

# Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C34209977&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C34209977&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>
<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>

# 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>mccvol:</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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