

# 2,4-Dichlorophenethylamine

<b>Inchi:</b>	InChI=1S/C8H9Cl2N/c9-7-2-1-6(3-4-11)8(10)5-7/h1-2,5H,3-4,11H2
<b>InchiKey:</b>	VHJKDOLGYMULOP-UHFFFAOYSA-N
<b>Formula:</b>	C8H9Cl2N
<b>SMILES:</b>	NCCc1ccc(Cl)cc1Cl
<b>Mol. weight [g/mol]:</b>	190.07
<b>CAS:</b>	52516-13-9

## Physical Properties

Property code	Value	Unit	Source
gf	152.22	kJ/mol	Joback Method
hf	7.45	kJ/mol	Joback Method
hfus	23.33	kJ/mol	Joback Method
hvap	56.41	kJ/mol	Joback Method
log10ws	-3.08		Crippen Method
logp	2.495		Crippen Method
mcvol	134.280	ml/mol	McGowan Method
pc	3452.08	kPa	Joback Method
tb	566.47	K	Joback Method
tc	801.63	K	Joback Method
tf	374.48	K	Joback Method
vc	0.502	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	276.02	J/molxK	566.47	Joback Method
cpg	286.70	J/molxK	605.66	Joback Method
cpg	296.67	J/molxK	644.86	Joback Method
cpg	305.96	J/molxK	684.05	Joback Method
cpg	314.60	J/molxK	723.24	Joback Method
cpg	322.63	J/molxK	762.44	Joback Method
cpg	330.07	J/molxK	801.63	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=C52516139&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C52516139&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.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>

# 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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