

# Alpha,alpha,alpha,2,4-pentachloroacetanilide

<b>Inchi:</b>	InChI=1S/C8H4Cl5NO/c9-4-1-2-6(5(10)3-4)14-7(15)8(11,12)13/h1-3H,(H,14,15)
<b>InchiKey:</b>	WGXCDDJEACXRNE-UHFFFAOYSA-N
<b>Formula:</b>	C8H4Cl5NO
<b>SMILES:</b>	O=C(Nc1ccc(Cl)cc1Cl)C(Cl)(Cl)Cl
<b>Mol. weight [g/mol]:</b>	307.39
<b>CAS:</b>	33560-54-2

## Physical Properties

Property code	Value	Unit	Source
gf	13.29	kJ/mol	Joback Method
hf	-141.42	kJ/mol	Joback Method
hfus	30.01	kJ/mol	Joback Method
hvap	70.81	kJ/mol	Joback Method
log10ws	-4.61		Crippen Method
logp	4.302		Crippen Method
mcvol	172.570	ml/mol	McGowan Method
pc	3173.97	kPa	Joback Method
tb	707.04	K	Joback Method
tc	963.68	K	Joback Method
tf	485.99	K	Joback Method
vc	0.650	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	340.50	J/mol×K	707.04	Joback Method
cpg	347.58	J/mol×K	749.81	Joback Method
cpg	353.89	J/mol×K	792.59	Joback Method
cpg	359.50	J/mol×K	835.36	Joback Method
cpg	364.51	J/mol×K	878.13	Joback Method
cpg	368.99	J/mol×K	920.90	Joback Method
cpg	373.03	J/mol×K	963.68	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=C33560542&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C33560542&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>
<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>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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