

# Alpha,alpha,alpha,2,4,5-hexachloroacetanilide

<b>Inchi:</b>	InChI=1S/C8H3Cl6NO/c9-3-1-5(11)6(2-4(3)10)15-7(16)8(12,13)14/h1-2H,(H,15,16)
<b>InchiKey:</b>	KTEQMHWNSTSS-UHFFFAOYSA-N
<b>Formula:</b>	C8H3Cl6NO
<b>SMILES:</b>	O=C(Nc1cc(Cl)c(Cl)cc1Cl)C(Cl)(Cl)Cl
<b>Mol. weight [g/mol]:</b>	341.83
<b>CAS:</b>	33560-57-5

## Physical Properties

Property code	Value	Unit	Source
gf	-8.27	kJ/mol	Joback Method
hf	-168.63	kJ/mol	Joback Method
hfus	33.82	kJ/mol	Joback Method
hvap	75.86	kJ/mol	Joback Method
log10ws	-5.29		Crippen Method
logp	4.956		Crippen Method
mcvol	184.810	ml/mol	McGowan Method
pc	2995.87	kPa	Joback Method
tb	749.45	K	Joback Method
tc	1008.70	K	Joback Method
tf	528.43	K	Joback Method
vc	0.700	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	354.72	J/molxK	749.45	Joback Method
cpg	360.70	J/molxK	792.66	Joback Method
cpg	366.00	J/molxK	835.87	Joback Method
cpg	370.71	J/molxK	879.08	Joback Method
cpg	374.91	J/molxK	922.28	Joback Method
cpg	378.67	J/molxK	965.49	Joback Method
cpg	382.07	J/molxK	1008.70	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=C33560575&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C33560575&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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