

# Bicyclo[2.2.1]hept-5-ene-2-carboxaldehyde, 1,4,5,6,7,7-hexachloro-

<b>Inchi:</b>	InChI=1S/C8H4Cl6O/c9-4-5(10)7(12)3(2-15)1-6(4,11)8(7,13)14/h2-3H,1H2
<b>InchiKey:</b>	JYYQMATWCIEKAT-UHFFFAOYSA-N
<b>Formula:</b>	C8H4Cl6O
<b>SMILES:</b>	O=CC1CC2(Cl)C(Cl)=C(Cl)C1(Cl)C2(Cl)Cl
<b>Mol. weight [g/mol]:</b>	328.83
<b>CAS:</b>	39234-24-7

## Physical Properties

Property code	Value	Unit	Source
gf	-66.41	kJ/mol	Joback Method
hf	-209.15	kJ/mol	Joback Method
hfus	21.81	kJ/mol	Joback Method
hvap	63.97	kJ/mol	Joback Method
log10ws	-4.59		Crippen Method
logp	4.037		Crippen Method
mcvol	172.570	ml/mol	McGowan Method
pc	3177.55	kPa	Joback Method
tb	673.93	K	Joback Method
tc	941.83	K	Joback Method
tf	522.82	K	Joback Method
vc	0.678	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	344.28	J/molxK	673.93	Joback Method
cpg	351.68	J/molxK	718.58	Joback Method
cpg	359.50	J/molxK	763.23	Joback Method
cpg	368.31	J/molxK	807.88	Joback Method
cpg	378.71	J/molxK	852.53	Joback Method
cpg	391.27	J/molxK	897.18	Joback Method
cpg	406.59	J/molxK	941.83	Joback Method

# Sources

<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=C39234247&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C39234247&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>

# 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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