

# Dienochlor

**Other names:**

1,1',2,2',3,3',4,4',5,5'-Decachlorobi-2,4-cyclopentadien-1-yl  
1,2,3,4,5-pentachloro-5-(1,2,3,4,5-pentachloro-1-cyclopenta-2,4-dienyl)cyclopenta-1,3-diene  
Bi-2,4-cyclopentadien-1-yl, 1,1',2,2',3,3',4,4',5,5'-decachloro-  
Bi-2,4-cyclopentadien-1-yl, decachloro-  
Bis(pentachlor-2,4-cyclopentadien-1-yl)  
Bis(pentachloro-2,4-cyclopentadien-1-yl)  
Bis(pentachlorocyclopentadienyl)  
Decachlor  
Decachlorobi-2,4-cyclopentadien-1-yl  
Decachlorobi-2,4-cyclopentadiene-1-yl  
Decachlorobis(2,4-cyclopentadiene-1-yl)  
Dienochlore  
ENT 25,718  
HRS 16  
HRS 1654  
HRS 16A  
Hooker HRS 1654  
Hooker HRS-16  
NSC 26106  
NSC 41880  
Pentac  
Pentac SP  
Pentac WP  
Pentac aquaflow

**Inchi:** InChI=1S/C10Cl10/c11-1-2(12)6(16)9(19,5(1)15)10(20)7(17)3(13)4(14)8(10)18  
**InchiKey:** LWLJUMBEZJHXHV-UHFFFAOYSA-N  
**Formula:** C10Cl10  
**SMILES:** ClC1=C(Cl)C(Cl)(C2(Cl)C(Cl)=C(Cl)C(Cl)=C2Cl)C(Cl)=C1Cl  
**Mol. weight [g/mol]:** 474.64  
**CAS:** 2227-17-0

## Physical Properties

Property code	Value	Unit	Source
gf	18.94	kJ/mol	Joback Method
hf	-116.33	kJ/mol	Joback Method
hfus	40.68	kJ/mol	Joback Method

hvap	86.38			kJ/mol	Joback Method
log10ws	-7.28				Aqueous Solubility Prediction Method
log10ws	-7.28				Estimated Solubility Method
logp	7.726				Crippen Method
mcvol	235.240			ml/mol	McGowan Method
pc	2324.78			kPa	Joback Method
tb	870.02			K	Joback Method
tc	1157.04			K	Joback Method
tf	674.46			K	Joback Method
vc	0.907			m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	416.13	J/mol×K	870.02	Joback Method
cpg	426.64	J/mol×K	917.86	Joback Method
cpg	439.17	J/mol×K	965.69	Joback Method
cpg	454.20	J/mol×K	1013.53	Joback Method
cpg	472.16	J/mol×K	1061.37	Joback Method
cpg	493.52	J/mol×K	1109.21	Joback Method
cpg	518.72	J/mol×K	1157.04	Joback Method

## Sources

**McGowan Method:**

<http://link.springer.com/article/10.1007/BF02311772>

**NIST Webbook:**

<http://webbook.nist.gov/cgi/cbook.cgi?ID=C2227170&Units=SI>

**Crippen Method:**

<http://pubs.acs.org/doi/abs/10.1021/ci9903071>

**Joback Method:**

[https://en.wikipedia.org/wiki/Joback\\_method](https://en.wikipedia.org/wiki/Joback_method)

**Aqueous Solubility Prediction Method:**

<http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa>

**Estimated Solubility Method:**

[http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl\\_file/ci034243xsi20040112\\_053635.txt](http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt)

## Legend

**cpg:** 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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