

# 1,3-Benzenedicarbonitrile, 4-methoxy-2,5,6-trichloro-

**Other names:** 4-Methoxy-2,5,6-trichloro-1,3-benzenedicarbonitrile

4-Methoxy-2,5,6-trichloroisophthalonitrile

2,4,5-Trichloro-6-methoxy-1,3-dicyanobenzene

Chlorthalonil, 4-methoxy

**Inchi:** InChI=1S/C9H3Cl3N2O/c1-15-9-5(3-14)6(10)4(2-13)7(11)8(9)12/h1H3

**InchiKey:** UXQSHXVXPDKJU-UHFFFAOYSA-N

**Formula:** C9H3Cl3N2O

**SMILES:** COc1c(Cl)c(Cl)c(C#N)c(Cl)c1C#N

**Mol. weight [g/mol]:** 261.49

**CAS:** 57531-87-0

## Physical Properties

Property code	Value	Unit	Source
gf	214.73	kJ/mol	Joback Method
hf	100.41	kJ/mol	Joback Method
hfus	27.95	kJ/mol	Joback Method
hvap	77.73	kJ/mol	Joback Method
log10ws	-4.35		Crippen Method
logp	3.399		Crippen Method
mcvol	159.260	ml/mol	McGowan Method
pc	2490.03	kPa	Joback Method
tb	795.77	K	Joback Method
tc	1044.96	K	Joback Method
tf	522.18	K	Joback Method
vc	0.648	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	322.95	J/molxK	795.77	Joback Method
cpg	328.79	J/molxK	837.30	Joback Method
cpg	334.08	J/molxK	878.83	Joback Method
cpg	338.80	J/molxK	920.36	Joback Method
cpg	342.93	J/molxK	961.89	Joback Method

cpg	346.46	J/mol×K	1003.43	Joback Method
cpg	349.36	J/mol×K	1044.96	Joback Method

## Sources

<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>
<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=C57531870&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C57531870&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>

## 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>hvac:</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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