

# Benzene, 1-chloro-4-(1-methylethenyl)-

<b>Other names:</b>	4-Chloro-«alpha»-methylstyrene p-Chloro-«alpha»-methylstyrene 4-ClC <sub>6</sub> H <sub>4</sub> C(CH <sub>3</sub> )=CH <sub>2</sub> 1-Chloro-4-isopropenylbenzene
<b>Inchi:</b>	InChI=1S/C <sub>9</sub> H <sub>9</sub> Cl/c1-7(2)8-3-5-9(10)6-4-8/h3-6H,1H <sub>2</sub> ,2H <sub>3</sub>
<b>InchiKey:</b>	WQDGTJOEMPEHHL-UHFFFAOYSA-N
<b>Formula:</b>	C <sub>9</sub> H <sub>9</sub> Cl
<b>SMILES:</b>	C=C(C)c1ccc(Cl)cc1
<b>Mol. weight [g/mol]:</b>	152.62
<b>CAS:</b>	1712-70-5

## Physical Properties

Property code	Value	Unit	Source
affp	854.30	kJ/mol	NIST Webbook
basg	825.40	kJ/mol	NIST Webbook
gf	195.04	kJ/mol	Joback Method
hf	95.87	kJ/mol	Joback Method
hfus	14.33	kJ/mol	Joback Method
hvap	42.36	kJ/mol	Joback Method
log10ws	-3.40		Crippen Method
logp	3.373		Crippen Method
mcvol	121.850	ml/mol	McGowan Method
pc	3243.03	kPa	Joback Method
rinpol	1146.00		NIST Webbook
tb	470.97	K	Joback Method
tc	695.36	K	Joback Method
tf	244.33	K	Joback Method
vc	0.463	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	225.88	J/mol×K	470.97	Joback Method
cpg	238.27	J/mol×K	508.37	Joback Method

cpg	249.85	J/mol×K	545.77	Joback Method
cpg	260.68	J/mol×K	583.16	Joback Method
cpg	270.79	J/mol×K	620.56	Joback Method
cpg	280.21	J/mol×K	657.96	Joback Method
cpg	288.99	J/mol×K	695.36	Joback Method

## Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C1712705&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C1712705&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>
<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>

## Legend

<b>affp:</b>	Proton affinity
<b>basg:</b>	Gas basicity
<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>rinpol:</b>	Non-polar retention indices
<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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