

# Benzene,1,2,3,4-tetrachloro-5-fluoro-

<b>Other names:</b>	1-Fluoro-2,3,4,5-tetrachlorobenzene
<b>Inchi:</b>	InChI=1S/C6HCl4F/c7-2-1-3(11)5(9)6(10)4(2)8/h1H
<b>InchiKey:</b>	ANICFDYFPBTMNX-UHFFFAOYSA-N
<b>Formula:</b>	C6HCl4F
<b>SMILES:</b>	Fc1cc(Cl)c(Cl)c(Cl)c1Cl
<b>Mol. weight [g/mol]:</b>	233.88
<b>CAS:</b>	2691-93-2

## Physical Properties

Property code	Value	Unit	Source
gf	-169.00	kJ/mol	Joback Method
hf	-235.59	kJ/mol	Joback Method
hfus	23.65	kJ/mol	Joback Method
hvap	50.60	kJ/mol	Joback Method
ie	9.20 ± 0.02	eV	NIST Webbook
log10ws	-4.54		Crippen Method
logp	4.439		Crippen Method
mcvol	122.370	ml/mol	McGowan Method
pc	3395.98	kPa	Joback Method
tb	532.27	K	Joback Method
tc	766.39	K	Joback Method
tf	354.15	K	Joback Method
vc	0.477	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	193.69	J/molxK	532.27	Joback Method
cpg	199.18	J/molxK	571.29	Joback Method
cpg	204.32	J/molxK	610.31	Joback Method
cpg	209.10	J/molxK	649.33	Joback Method
cpg	213.56	J/molxK	688.35	Joback Method
cpg	217.69	J/molxK	727.37	Joback Method
cpg	221.51	J/molxK	766.39	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=C2691932&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C2691932&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.cheméo.com/doc/models/crippen_log10ws">https://www.cheméo.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>ie:</b>	Ionization energy
<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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