

# 1-Chloro-2,5-difluorobenzene

Other names:	Benzene,2-chloro-1,4-difluoro-
Inchi:	InChI=1S/C6H3ClF2/c7-5-3-4(8)1-2-6(5)9/h1-3H
InchiKey:	XWCKSJOUZQHFKE-UHFFFAOYSA-N
Formula:	C6H3ClF2
SMILES:	Fc1ccc(F)c(Cl)c1
Mol. weight [g/mol]:	148.54
CAS:	2367-91-1

## Physical Properties

Property code	Value	Unit	Source
gf	-308.76	kJ/mol	Joback Method
hf	-361.54	kJ/mol	Joback Method
hfus	14.92	kJ/mol	Joback Method
hvap	35.30	kJ/mol	Joback Method
ie	9.19 ± 0.02	eV	NIST Webbook
log10ws	-2.82		Crippen Method
logp	2.618		Crippen Method
mcvol	87.420	ml/mol	McGowan Method
pc	3810.39	kPa	Joback Method
tb	409.29	K	Joback Method
tc	610.29	K	Joback Method
tf	239.94	K	Joback Method
vc	0.348	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	144.97	J/molxK	409.29	Joback Method
cpg	152.39	J/molxK	442.79	Joback Method
cpg	159.40	J/molxK	476.29	Joback Method
cpg	166.03	J/molxK	509.79	Joback Method
cpg	172.28	J/molxK	543.29	Joback Method
cpg	178.17	J/molxK	576.79	Joback Method
cpg	183.71	J/molxK	610.29	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=C2367911&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C2367911&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>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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