

# C6H3Cl2FO2S

<b>Inchi:</b>	InChI=1S/C6H3Cl2FO2S/c7-5-3-4(12(8,10)11)1-2-6(5)9/h1-3H
<b>InchiKey:</b>	DXFXNSNBZNELII-UHFFFAOYSA-N
<b>Formula:</b>	C6H3Cl2FO2S
<b>SMILES:</b>	O=S(=O)(Cl)c1ccc(F)c(Cl)c1
<b>Mol. weight [g/mol]:</b>	229.06
<b>CAS:</b>	91170-93-3

## Physical Properties

Property code	Value	Unit	Source
gf	-594.42	kJ/mol	Joback Method
hf	-634.52	kJ/mol	Joback Method
hfus	27.41	kJ/mol	Joback Method
hvap	59.14	kJ/mol	Joback Method
log10ws	-2.91		Crippen Method
logp	2.407		Crippen Method
mcvol	125.980	ml/mol	McGowan Method
pc	4710.65	kPa	Joback Method
tb	495.23	K	Joback Method
tc	707.91	K	Joback Method
tf	307.83	K	Joback Method
vc	0.505	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	225.24	J/molxK	495.23	Joback Method
cpg	233.59	J/molxK	530.68	Joback Method
cpg	241.45	J/molxK	566.12	Joback Method
cpg	248.81	J/molxK	601.57	Joback Method
cpg	255.68	J/molxK	637.02	Joback Method
cpg	262.05	J/molxK	672.46	Joback Method
cpg	267.91	J/molxK	707.91	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=C91170933&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C91170933&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</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>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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