2-Chloro-4-fluorobenzenesulphonyl chloride

Inchi: InChI=1S/C6H3Cl2FO2S/c7-5-3-4(9)1-2-6(5)12(8,10)11/h1-3H
InchiKey: FCFPJKHVCHKCMP-UHFFFAOYSA-N
Formula: C6H3Cl2FO2S
SMILES: O=S(=O)(Cl)c1ccc(F)cc1Cl
Mol. weight [g/mol]: 229.06
CAS: 85958-57-2

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/mol×K	495.23	Joback Method
cpg	233.59	J/mol×K	530.68	Joback Method
cpg	241.45	J/mol×K	566.12	Joback Method
cpg	248.81	J/mol×K	601.57	Joback Method
cpg	255.68	J/mol×K	637.02	Joback Method
cpg	262.05	J/mol×K	672.46	Joback Method
cpg	267.91	J/mol×K	707.91	Joback Method

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C85958572&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume