3-Chlorobenzenesulfonyl chloride

Other names: Benzenesulfonyl chloride, 3-chloro-
3-chlorobenzenesulphonyl chloride
Inchi: InChI=1S/C6H4Cl2O2S/c7-5-2-1-3-6(4-5)11(8,9)10/h1-4H
InchiKey: OINWZUJVEXUHCC-UHFFFAOYSA-N
Formula: C6H4Cl2O2S
SMILES: O=S(=O)(Cl)c1cccc(Cl)c1
Mol. weight [g/mol]: 211.07
CAS: 2888-06-4

Physical Properties

Property code	Value	Unit	Source
gf	-389.98	kJ/mol	Joback Method
hf	-426.94	kJ/mol	Joback Method
hfus	24.72	kJ/mol	Joback Method
hvap	59.29	kJ/mol	Joback Method
log10ws	-2.57		Crippen Method
logp	2.268		Crippen Method
mcvol	124.210	ml/mol	McGowan Method
pc	5123.98	kPa	Joback Method
tb	490.98	K	Joback Method
tc	714.16	K	Joback Method
tf	294.72	K	Joback Method
vc	0.487	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	217.31	J/mol×K	490.98	Joback Method
cpg	226.54	J/mol×K	528.18	Joback Method
cpg	235.17	J/mol×K	565.37	Joback Method
cpg	243.20	J/mol×K	602.57	Joback Method
cpg	250.65	J/mol×K	639.77	Joback Method
cpg	257.50	J/mol×K	676.96	Joback Method
cpg	263.77	J/mol×K	714.16	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=C2888064&Units=SI

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