3-Chlorobenzenesulfonamide

Other names:	Benzenesulfonamide, 3-chloro-
Inchi:	InChI=1S/C6H6ClNO2S/c7-5-2-1-3-6(4-5)11(8,9)10/h1-4H,(H2,8,9,10)
InchiKey:	WSYQJNPRQUFCGL-UHFFFAOYSA-N
Formula:	C6H6ClNO2S
SMILES:	NS(=O)(=O)c1cccc(Cl)c1
Mol. weight [g/mol]:	191.63
CAS:	17260-71-8

Physical Properties

Property code	Value	Unit	Source
gf	-311.60	kJ/mol	Joback Method
hf	-377.41	kJ/mol	Joback Method
hfus	25.72	kJ/mol	Joback Method
hvap	65.55	kJ/mol	Joback Method
log10ws	-1.86		Crippen Method
logp	0.987		Crippen Method
mcvol	121.950	ml/mol	McGowan Method
pc	5889.94	kPa	Joback Method
tb	526.08	K	Joback Method
tc	754.53	K	Joback Method
tf	348.06	K	Joback Method
vc	0.468	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	242.55	J/mol×K	526.08	Joback Method
cpg	252.62	J/mol×K	564.16	Joback Method
cpg	262.01	J/mol×K	602.23	Joback Method
cpg	270.72	J/mol×K	640.31	Joback Method
cpg	278.77	J/mol×K	678.38	Joback Method
cpg	286.15	J/mol×K	716.46	Joback Method
cpg	292.87	J/mol×K	754.53	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=C17260718&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

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