2,3-Dichlorobenzenethiol

Other names: 2,3-Dichlorothiophenol
Benzenethiol, 2,3-dichloro-
Inchi: InChI=1S/C6H4Cl2S/c7-4-2-1-3-5(9)6(4)8/h1-3,9H
InchiKey: QGRKONUHHGBHRB-UHFFFAOYSA-N
Formula: C6H4Cl2S
SMILES: Sc1cccc(Cl)c1Cl
Mol. weight [g/mol]: 179.07
CAS: 17231-95-7

Physical Properties

Property code	Value	Unit	Source
gf	98.32	kJ/mol	Joback Method
hf	53.42	kJ/mol	Joback Method
hfus	17.00	kJ/mol	Joback Method
hvap	48.06	kJ/mol	Joback Method
log10ws	-3.36		Crippen Method
logp	3.282		Crippen Method
mcvol	112.470	ml/mol	McGowan Method
pc	4426.72	kPa	Joback Method
tb	511.04	K	Joback Method
tc	769.63	K	Joback Method
tf	305.14	K	Joback Method
vc	0.415	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	185.08	J/mol×K	511.04	Joback Method
cpg	193.15	J/mol×K	554.14	Joback Method
cpg	200.62	J/mol×K	597.24	Joback Method
cpg	207.51	J/mol×K	640.34	Joback Method
cpg	213.84	J/mol×K	683.44	Joback Method
cpg	219.66	J/mol×K	726.54	Joback Method
cpg	224.97	J/mol×K	769.63	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=C17231957&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