

4-Chlorobenzenesulfonic acid

Other names:	p-Chlorobenzenesulfonic acid Benzenesulfonic acid, 4-chloro- 4-chlorobenzenesulphonic acid
Inchi:	InChI=1S/C6H5ClO3S/c7-5-1-3-6(4-2-5)11(8,9)10/h1-4H,(H,8,9,10)
InchiKey:	RJWBTWIBUIGANW-UHFFFAOYSA-N
Formula:	C6H5ClO3S
SMILES:	O=S(=O)(O)c1ccc(Cl)cc1
Mol. weight [g/mol]:	192.62
CAS:	98-66-8

Physical Properties

Property code	Value	Unit	Source
gf	-514.87	kJ/mol	Joback Method
hf	-563.43	kJ/mol	Joback Method
hfus	24.61	kJ/mol	Joback Method
hvap	71.59	kJ/mol	Joback Method
log10ws	-1.75		Crippen Method
logp	1.587		Crippen Method
mcvol	117.840	ml/mol	McGowan Method
pc	6219.59	kPa	Joback Method
tb	545.73	K	Joback Method
tc	748.41	K	Joback Method
tf	325.62	K	Joback Method
vc	0.458	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	264.72	J/mol×K	680.85	Joback Method
cpg	270.87	J/mol×K	714.63	Joback Method
cpg	235.08	J/mol×K	545.73	Joback Method
cpg	243.25	J/mol×K	579.51	Joback Method
cpg	250.91	J/mol×K	613.29	Joback Method
cpg	258.07	J/mol×K	647.07	Joback Method

cpg	276.53	J/mol×K	748.41	Joback Method
hfust	10.60	kJ/mol	333.20	NIST Webbook
hfust	10.60	kJ/mol	333.20	NIST Webbook

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=C98668&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
hfust:	Enthalpy of fusion at a given temperature
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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