4-CHLOROBENZENESULPHONIC 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

Physical Properties

Property code	Value	Unit	Source
hf	-449.36	kJ/mol	Cheméo Relay (1.0)
hfus	24.61	kJ/mol	Joback Method
hvap	106.90	kJ/mol	Cheméo Relay (1.0)
ie	9.85	eV	Cheméo Relay (1.0)
log10ws	-0.98		Cheméo Relay (1.0)
logp	1.587		Crippen Method
mcvol	117.840	ml/mol	McGowan Method
tb	563.80	K	Cheméo Relay (1.0)
tf	518.84	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
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	264.72	J/mol×K	680.85	Joback Method
cpg	270.87	J/mol×K	714.63	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:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C98668&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

cpg:	Ideal gas heat capacity
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
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point