

1,2-Benzenediol, 4-chloro-

Other names:	Pyrocatechol, 4-chloro- 4-Chlorocatechol 4-Chloropyrocatechol 4-Chloro-benzene-1,2-diol 4-Chloro-1,2-benzenediol
Inchi:	InChI=1S/C6H5ClO2/c7-4-1-2-5(8)6(9)3-4/h1-3,8-9H
InchiKey:	WWOBYPKUYODHDG-UHFFFAOYSA-N
Formula:	C6H5ClO2
SMILES:	Oc1ccc(Cl)cc1O
Mol. weight [g/mol]:	144.56
CAS:	2138-22-9

Physical Properties

Property code	Value	Unit	Source
gf	-209.12	kJ/mol	Joback Method
hf	-301.00	kJ/mol	Joback Method
hfus	21.10	kJ/mol	Joback Method
hvap	61.64	kJ/mol	Joback Method
log10ws	-1.25		Crippen Method
logp	1.751		Crippen Method
mcvol	95.620	ml/mol	McGowan Method
pc	6921.35	kPa	Joback Method
tb	562.03	K	Joback Method
tc	814.87	K	Joback Method
tf	437.16	K	Joback Method
vc	0.244	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	238.99	J/molxK	814.87	Joback Method
cpg	204.56	J/molxK	562.03	Joback Method
cpg	211.65	J/molxK	604.17	Joback Method
cpg	217.98	J/molxK	646.31	Joback Method

cpg	223.72	J/mol×K	688.45	Joback Method
cpg	229.02	J/mol×K	730.59	Joback Method
cpg	234.06	J/mol×K	772.73	Joback Method
dvisc	0.0000140	Paxs	562.03	Joback Method
dvisc	0.0003117	Paxs	437.16	Joback Method
dvisc	0.0001652	Paxs	457.97	Joback Method
dvisc	0.0000925	Paxs	478.78	Joback Method
dvisc	0.0000544	Paxs	499.60	Joback Method
dvisc	0.0000334	Paxs	520.41	Joback Method
dvisc	0.0000213	Paxs	541.22	Joback Method
hvapt	70.20	kJ/mol	308.00	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=C2138229&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
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
hvapt:	Enthalpy of vaporization at a given temperature
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mvol:	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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