

1,3-Benzenediol, 4-chloro-

Other names:	Resorcinol, 4-chloro- p-Chlororesorcinol C.I. 76510 4-Chloro-1,3-Benzenediol 4-Chloro-1,3-dihydroxybenzene 4-Chlororesorcinol
Inchi:	InChI=1S/C6H5ClO2/c7-5-2-1-4(8)3-6(5)9/h1-3,8-9H
InchiKey:	JQVAPEJNIZULEK-UHFFFAOYSA-N
Formula:	C6H5ClO2
SMILES:	Oc1ccc(Cl)c(O)c1
Mol. weight [g/mol]:	144.56
CAS:	95-88-5

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	204.56	J/mol×K	562.03	Joback Method
cpg	211.65	J/mol×K	604.17	Joback Method
cpg	217.98	J/mol×K	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
cpg	238.99	J/mol×K	814.87	Joback Method
dvisc	0.0003117	Pa×s	437.16	Joback Method
dvisc	0.0001652	Pa×s	457.97	Joback Method
dvisc	0.0000925	Pa×s	478.78	Joback Method
dvisc	0.0000544	Pa×s	499.60	Joback Method
dvisc	0.0000334	Pa×s	520.41	Joback Method
dvisc	0.0000213	Pa×s	541.22	Joback Method
dvisc	0.0000140	Pa×s	562.03	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	420.20	K	2.40	NIST Webbook

Sources

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=C95885&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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
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
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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