

1,4-Benzenediol, 2-chloro-

Other names:	Hydroquinone, chloro- Chlorohydroquinone 1,4-Dihydroxy-2-chlorobenzene 2-Chloro-1,4-benzenediol 2-Chlorohydroquinone Chloroquinol Monochlorohydroquinone 2-Chloro-1,4-dihydroxybenzene NSC 427 NSC 5934
Inchi:	InChI=1S/C6H5ClO2/c7-5-3-4(8)1-2-6(5)9/h1-3,8-9H
InchiKey:	AJPXTSMULZANCB-UHFFFAOYSA-N
Formula:	C6H5ClO2
SMILES:	Oc1ccc(O)c(Cl)c1
Mol. weight [g/mol]:	144.56
CAS:	615-67-8

Physical Properties

Property code	Value	Unit	Source
chs	-2702.00	kJ/mol	NIST Webbook
chs	-2714.00	kJ/mol	NIST Webbook
chs	-2716.30 ± 8.40	kJ/mol	NIST Webbook
gf	-209.12	kJ/mol	Joback Method
hf	-301.00	kJ/mol	Joback Method
hfs	-393.00	kJ/mol	NIST Webbook
hfus	21.10	kJ/mol	Joback Method
hsub	102.93	kJ/mol	NIST Webbook
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	536.20	K	NIST Webbook
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/mol×K	814.87	Joback Method
cpg	234.06	J/mol×K	772.73	Joback Method
cpg	229.02	J/mol×K	730.59	Joback Method
cpg	223.72	J/mol×K	688.45	Joback Method
cpg	217.98	J/mol×K	646.31	Joback Method
cpg	211.65	J/mol×K	604.17	Joback Method
cpg	204.56	J/mol×K	562.03	Joback Method
dvisc	0.0003117	Pa×s	437.16	Joback Method
dvisc	0.0000140	Pa×s	562.03	Joback Method
dvisc	0.0000213	Pa×s	541.22	Joback Method
dvisc	0.0000334	Pa×s	520.41	Joback Method
dvisc	0.0000544	Pa×s	499.60	Joback Method
dvisc	0.0000925	Pa×s	478.78	Joback Method
dvisc	0.0001652	Pa×s	457.97	Joback Method
hsubt	102.90 ± 8.30	kJ/mol	320.00	NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C615678&Units=SI
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

Legend

chs:	Standard solid enthalpy of combustion
cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions

hfs:	Solid phase enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hsub:	Enthalpy of sublimation at standard conditions
hsubt:	Enthalpy of sublimation 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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