2,6-dichlorohydroquinone

Other names: 2,6-Dichloro-1,4-benzenediol
Inchi: InChI=1S/C6H4Cl2O2/c7-4-1-3(9)2-5(8)6(4)10/h1-2,9-10H
InchiKey: QQAHQUBHRBQWBL-UHFFFAOYSA-N
Formula: C6H4Cl2O2
SMILES: Oc1cc(Cl)c(O)c(Cl)c1
Mol. weight [g/mol]: 179.00
CAS: 20103-10-0

Physical Properties

Property code	Value	Unit	Source
chs	-2569.00	kJ/mol	NIST Webbook
chs	-2551.00	kJ/mol	NIST Webbook
chs	-2556.40 ± 8.40	kJ/mol	NIST Webbook
gf	-230.68	kJ/mol	Joback Method
hf	-328.21	kJ/mol	Joback Method
hfs	-433.90	kJ/mol	NIST Webbook
hfus	24.91	kJ/mol	Joback Method
hsub	92.05	kJ/mol	NIST Webbook
hvap	66.69	kJ/mol	Joback Method
log10ws	-1.94		Crippen Method
logp	2.405		Crippen Method
mcvol	107.860	ml/mol	McGowan Method
pc	6359.24	kPa	Joback Method
tb	604.44	K	Joback Method
tc	861.92	K	Joback Method
tf	479.60	K	Joback Method
vc	0.293	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	220.56	J/mol×K	604.44	Joback Method
cpg	226.43	J/mol×K	647.35	Joback Method
cpg	231.76	J/mol×K	690.27	Joback Method

cpg	236.70	J/mol×K	733.18	Joback Method
cpg	241.40	J/mol×K	776.09	Joback Method
cpg	246.05	J/mol×K	819.00	Joback Method
cpg	250.80	J/mol×K	861.92	Joback Method
dvisc	0.0001179	Pa×s	479.60	Joback Method
dvisc	0.0000687	Pa×s	500.41	Joback Method
dvisc	0.0000418	Pa×s	521.21	Joback Method
dvisc	0.0000264	Pa×s	542.02	Joback Method
dvisc	0.0000173	Pa×s	562.83	Joback Method
dvisc	0.0000117	Pa×s	583.63	Joback Method
dvisc	0.0000081	Pa×s	604.44	Joback Method
hsubt	92.00 ± 8.30	kJ/mol	334.50	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	2.53499e+01
Coeff. B	-1.09499e+04
Temperature range (K), min.	436.90
Temperature range (K), max.	546.44

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=C20103100&Units=SI

The Yaws Handbook of Vapor Pressure: https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
pvap:	Vapor pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume