Phenol, 2,4-dichloro-

Other names:	1,3-Dichloro-4-hydroxybenzene
	1-Hydroxy-2,4-dichlorobenzene
	2,4-DCP
	2,4-Dichlorophenol
	4,6-Dichlorophenol
	DCP
	NCI-C55345
	NSC 2879
	Rcra waste number U081
Inchi:	InChI=1S/C6H4Cl2O/c7-4-1-2-6(9)5(8)3-4/h1-3,9H
InchiKey:	HFZWRUODUSTPEG-UHFFFAOYSA-N
Formula:	C6H4Cl2O
SMILES:	Oc1ccc(Cl)cc1Cl
Mol. weight [g/mol]:	163.00
CAS:	120-83-2

Physical Properties

Property code	Value	Unit	Source
chs	-2753.70 ± 1.30	kJ/mol	NIST Webbook
gf	-76.06	kJ/mol	Joback Method
hf	-156.30 ± 1.90	kJ/mol	NIST Webbook
hfs	-226.40 ± 1.50	kJ/mol	NIST Webbook
hfus	19.13	kJ/mol	Joback Method
hsub	70.10 ± 1.10	kJ/mol	NIST Webbook
hsub	70.10 ± 1.10	kJ/mol	NIST Webbook
hsub	78.00 ± 0.30	kJ/mol	NIST Webbook
hvap	58.10 ± 0.30	kJ/mol	NIST Webbook
hvap	59.00 ± 0.40	kJ/mol	NIST Webbook
log10ws	-1.55		Estimated Solubility Method
log10ws	-1.55		Aqueous Solubility Prediction Method
logp	2.699		Crippen Method
mcvol	101.990	ml/mol	McGowan Method
pc	5080.25	kPa	Joback Method
rinpol	1189.00		NIST Webbook
rinpol	1140.00		NIST Webbook

rinpol	1140.00	NIST Webbook
rinpol	1144.00	NIST Webbook
rinpol	196.30	NIST Webbook
rinpol	196.53	NIST Webbook
rinpol	1183.00	NIST Webbook
rinpol	1187.70	NIST Webbook
rinpol	1188.00	NIST Webbook
rinpol	1183.00	NIST Webbook
rinpol	1170.00	NIST Webbook
rinpol	1165.00	NIST Webbook
rinpol	1160.00	NIST Webbook
rinpol	1170.00	NIST Webbook
rinpol	1181.00	NIST Webbook
rinpol	1170.00	NIST Webbook
rinpol	1183.00	NIST Webbook
rinpol	1144.80	NIST Webbook
rinpol	1151.00	NIST Webbook
rinpol	1148.00	NIST Webbook
rinpol	1169.00	NIST Webbook
rinpol	1156.00	NIST Webbook
rinpol	1165.00	NIST Webbook
rinpol	1168.00	NIST Webbook
rinpol	1147.00	NIST Webbook
rinpol	1158.00	NIST Webbook
rinpol	1187.70	NIST Webbook
rinpol	1164.00	NIST Webbook
rinpol	1165.00	NIST Webbook
rinpol	1138.00	NIST Webbook
rinpol	1143.00	NIST Webbook
rinpol	1163.00	NIST Webbook
rinpol	1188.00	NIST Webbook
rinpol	1193.00	NIST Webbook
rinpol	1160.00	NIST Webbook
rinpol	1189.00	NIST Webbook
rinpol	1164.00	NIST Webbook
ripol	2151.00	NIST Webbook
ripol	2098.00	NIST Webbook
ripol	2096.00	NIST Webbook
ripol	2192.93	NIST Webbook
ripol	2098.00	NIST Webbook
ripol	2098.00	NIST Webbook
ripol	2104.00	NIST Webbook
ripol	2096.00	NIST Webbook
ripol	2120.00	NIST Webbook

ripol	2182.99		NIST Webbook
ripol	2151.00		NIST Webbook
ripol	2184.21		NIST Webbook
ripol	2192.93		NIST Webbook
ripol	2145.00		NIST Webbook
ripol	2131.00		NIST Webbook
ripol	2192.08		NIST Webbook
tb	483.20	K	NIST Webbook
tc	770.43	K	Joback Method
tf	316.65	K	Aqueous Solubility Prediction Method
tf	318.00 ± 0.20	K	NIST Webbook
tf	323.00 ± 2.00	K	NIST Webbook
tf	318.00 ± 3.00	K	NIST Webbook
vc	0.328	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	186.59	J/mol×K	523.82	Joback Method
cpg	200.54	J/mol×K	606.02	Joback Method
cpg	206.57	J/mol×K	647.12	Joback Method
cpg	212.08	J/mol×K	688.23	Joback Method
cpg	217.16	J/mol×K	729.33	Joback Method
cpg	221.90	J/mol×K	770.43	Joback Method
cpg	193.91	J/mol×K	564.92	Joback Method
dvisc	0.0003059	Pa×s	445.85	Joback Method
dvisc	0.0001933	Pa×s	471.84	Joback Method
dvisc	0.0009180	Pa×s	393.87	Joback Method
dvisc	0.0017868	Pa×s	367.88	Joback Method
dvisc	0.0001282	Pa×s	497.83	Joback Method
dvisc	0.0000885	Pa×s	523.82	Joback Method
dvisc	0.0005122	Pa×s	419.86	Joback Method
hfust	20.09	kJ/mol	318.00	NIST Webbook
hfust	20.09	kJ/mol	318.00	NIST Webbook
hfust	20.09	kJ/mol	318.00	NIST Webbook
hfust	28.41	kJ/mol	323.00	NIST Webbook
hvapt	56.60	kJ/mol	330.50	NIST Webbook
hvapt	52.30	kJ/mol	383.00	NIST Webbook
hvapt	60.80	kJ/mol	404.50	NIST Webbook
hvapt	36.78	kJ/mol	491.00	NIST Webbook

psub	0.01	kPa	297.30	Thermochemistry of Chlorobenzenes and Chlorophenols: Ambient Temperature Vapor Pressures and Enthalpies of Phase Transitions	
psub	0.05	kPa	309.40	Thermochemistry of Chlorobenzenes and Chlorophenols: Ambient Temperature Vapor Pressures and Enthalpies of Phase Transitions	
psub	0.04	kPa	306.30	Thermochemistry of Chlorobenzenes and Chlorophenols: Ambient Temperature Vapor Pressures and Enthalpies of Phase Transitions	
psub	0.03	kPa	303.30	Thermochemistry of Chlorobenzenes and Chlorophenols: Ambient Temperature Vapor Pressures and Enthalpies of Phase Transitions	
psub	0.02	kPa	300.40	Thermochemistry of Chlorobenzenes and Chlorophenols: Ambient Temperature Vapor Pressures and Enthalpies of Phase Transitions	

psub	0.07	kPa	312.40	Thermochemistry of Chlorobenzenes and Chlorophenols: Ambient Temperature Vapor Pressures and Enthalpies of Phase Transitions	
psub	0.01	kPa	294.40	Thermochemistry of Chlorobenzenes and Chlorophenols: Ambient Temperature Vapor Pressures and Enthalpies of Phase Transitions	
psub	6.26e-03	kPa	289.30	Thermochemistry of Chlorobenzenes and Chlorophenols: Ambient Temperature Vapor Pressures and Enthalpies of Phase Transitions	
psub	3.12e-03	kPa	283.30	Thermochemistry of Chlorobenzenes and Chlorophenols: Ambient Temperature Vapor Pressures and Enthalpies of Phase Transitions	
psub	1.75e-03	kPa	278.20	Thermochemistry of Chlorobenzenes and Chlorophenols: Ambient Temperature Vapor Pressures and Enthalpies of Phase Transitions	

psub	0.09	kPa	315.20	Thermochemistry of Chlorobenzenes and Chlorophenols: Ambient Temperature Vapor Pressures and Enthalpies of Phase Transitions
sfust	63.18	J/mol×K	318.00	NIST Webbook
sfust	88.00	J/mol×K	323.00	NIST Webbook
svapt	74.90	J/mol×K	491.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.50381e+01
Coeff. B	-4.81365e+03
Coeff. C	-3.99350e+01
Temperature range (K), min.	326.00
Temperature range (K), max.	534.83

Sources

The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
Thermochemistry of Chlorobenzenes and Chlorophenols: Ambient Temperature Vapor Pressures and Enthalpies of Phase Transitions:	https://www.doi.org/10.1021/je060429r
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
Solubilities of Some Chlorophenols in Supercritical CO2 in the Presence and Absence of Cosolvents:	https://www.doi.org/10.1021/je900328c
Estimated Solubility Method:	http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C120832&Units=SI
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
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
hfust:	Enthalpy of fusion at a given temperature
hsub:	Enthalpy of sublimation 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
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
psub:	Sublimation pressure
pvap:	Vapor pressure
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
sfust:	Entropy of fusion at a given temperature
svapt:	Entropy of vaporization at a given temperature
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume