Phenol, 2,6-dichloro-

Other names:	2,6-Dichlorfenol
	2,6-Dichlorophenol
	Rcra waste number U082
Inchi:	InChI=1S/C6H4Cl2O/c7-4-2-1-3-5(8)6(4)9/h1-3,9H
InchiKey:	HOLHYSJJBXSLMV-UHFFFAOYSA-N
Formula:	C6H4Cl2O
SMILES:	Oc1c(Cl)cccc1Cl
Mol. weight [g/mol]:	163.00
CAS:	87-65-0

Physical Properties

Property code	Value	Unit	Source
chs	-2758.00 ± 0.70	kJ/mol	NIST Webbook
gf	-76.06	kJ/mol	Joback Method
hf	-146.30 ± 1.50	kJ/mol	NIST Webbook
hfs	-222.10 ± 1.10	kJ/mol	NIST Webbook
hfus	19.13	kJ/mol	Joback Method
hsub	75.80 ± 1.00	kJ/mol	NIST Webbook
hsub	79.30 ± 0.20	kJ/mol	NIST Webbook
hsub	75.80 ± 1.10	kJ/mol	NIST Webbook
hvap	58.50 ± 0.50	kJ/mol	NIST Webbook
hvap	59.60 ± 0.30	kJ/mol	NIST Webbook
ie	8.65 ± 0.02	eV	NIST Webbook
log10ws	-1.79		Aqueous Solubility Prediction Method
log10ws	-1.79		Estimated Solubility Method
logp	2.699		Crippen Method
mcvol	101.990	ml/mol	McGowan Method
pc	5080.25	kPa	Joback Method
rinpol	1198.00		NIST Webbook
rinpol	1227.00		NIST Webbook
rinpol	1228.00		NIST Webbook
rinpol	1206.00		NIST Webbook
rinpol	1189.00		NIST Webbook
rinpol	1214.00		NIST Webbook
rinpol	1168.00		NIST Webbook
rinpol	1179.00		NIST Webbook

rinpol	1178.00		NIST Webbook
rinpol	1151.00		NIST Webbook
rinpol	1149.00		NIST Webbook
rinpol	1199.00		NIST Webbook
rinpol	204.68		NIST Webbook
rinpol	1223.20		NIST Webbook
rinpol	1190.00		NIST Webbook
rinpol	1200.00		NIST Webbook
rinpol	1194.00		NIST Webbook
rinpol	1189.00		NIST Webbook
rinpol	1200.00		NIST Webbook
rinpol	1179.00		NIST Webbook
rinpol	1203.00		NIST Webbook
rinpol	1206.00		NIST Webbook
rinpol	1205.00		NIST Webbook
rinpol	1213.00		NIST Webbook
rinpol	203.40		NIST Webbook
ripol	2097.00		NIST Webbook
ripol	2119.00		NIST Webbook
ripol	2097.00		NIST Webbook
ripol	2061.00		NIST Webbook
ripol	2124.00		NIST Webbook
ripol	2119.00		NIST Webbook
ripol	2083.00		NIST Webbook
ripol	2081.00		NIST Webbook
ripol	2038.00		NIST Webbook
ripol	2097.00		NIST Webbook
tb	492.20	K	NIST Webbook
tc	770.43	K	Joback Method
tf	340.00 ± 0.20	K	NIST Webbook
tf	340.90	K	Aqueous Solubility Prediction Method
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	0.0005122	Pa×s	419.86	Joback Method
dvisc	0.0017868	Pa×s	367.88	Joback Method
dvisc	0.0003059	Pa×s	445.85	Joback Method
dvisc	0.0001933	Pa×s	471.84	Joback Method
dvisc	0.0001282	Pa×s	497.83	Joback Method
dvisc	0.0000885	Pa×s	523.82	Joback Method
dvisc	0.0009180	Pa×s	393.87	Joback Method
hfust	22.14	kJ/mol	340.00	NIST Webbook
hfust	22.14	kJ/mol	340.00	NIST Webbook
hvapt	55.40	kJ/mol	356.00	NIST Webbook
hvapt	51.60	kJ/mol	400.00	NIST Webbook
hvapt	57.90	kJ/mol	413.00	NIST Webbook
psub	0.02	kPa	310.40	Thermochemistry of Chlorobenzenes and Chlorophenols: Ambient Temperature Vapor Pressures and Enthalpies of Phase Transitions
psub	0.08	kPa	322.40	Thermochemistry of Chlorobenzenes and Chlorophenols: Ambient Temperature Vapor Pressures and Enthalpies of Phase Transitions
psub	0.06	kPa	319.40	Thermochemistry of Chlorobenzenes and Chlorophenols: Ambient Temperature Vapor Pressures and Enthalpies of Phase Transitions

psub	0.04	kPa	316.40	Thermochemistry of Chlorobenzenes and Chlorophenols: Ambient Temperature Vapor Pressures and Enthalpies of Phase Transitions	
psub	0.03	kPa	313.40	Thermochemistry of Chlorobenzenes and Chlorophenols: Ambient Temperature Vapor Pressures and Enthalpies of Phase Transitions	
psub	0.10	kPa	325.40	Thermochemistry of Chlorobenzenes and Chlorophenols: Ambient Temperature Vapor Pressures and Enthalpies of Phase Transitions	
psub	0.02	kPa	307.40	Thermochemistry of Chlorobenzenes and Chlorophenols: Ambient Temperature Vapor Pressures and Enthalpies of Phase Transitions	
psub	0.01	kPa	304.60	Thermochemistry of Chlorobenzenes and Chlorophenols: Ambient Temperature Vapor Pressures and Enthalpies of Phase Transitions	

psub	0.01	kPa	301.60	Thermochemistry of Chlorobenzenes and Chlorophenols: Ambient Temperature Vapor Pressures and Enthalpies of Phase Transitions
psub	7.30e-03	kPa	298.50	Thermochemistry of Chlorobenzenes and Chlorophenols: Ambient Temperature Vapor Pressures and Enthalpies of Phase Transitions
psub	0.13	kPa	328.40	Thermochemistry of Chlorobenzenes and Chlorophenols: Ambient Temperature Vapor Pressures and Enthalpies of Phase Transitions
psub	0.17	kPa	331.30	Thermochemistry of Chlorobenzenes and Chlorophenols: Ambient Temperature Vapor Pressures and Enthalpies of Phase Transitions
sfust	65.12	J/mol×K	340.00	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	355.70	K	0.50	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.60385e+01
Coeff. B	-5.31628e+03
Coeff. C	-3.63910e+01
Temperature range (K), min.	333.00
Temperature range (K), max.	531.99

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C87650&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
Thermochemistry of Chlorobenzenes and Chlorophenols: Ambient Temperature Vapor Pressures and Enthalpies of Phase Transitions:	https://www.doi.org/10.1021/je060429r
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
Estimated Solubility Method:	http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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
ie:	Ionization energy

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