Phenol, 3,4-dichloro-

Other names: 3,4-Dichlorophenol
4,5-Dichlorophenol
Inchi: InChI=1S/C6H4Cl2O/c7-5-2-1-4(9)3-6(5)8/h1-3,9H
InchiKey: WDNBURPWRNALGP-UHFFFAOYSA-N
Formula: C6H4Cl2O
SMILES: Oc1ccc(Cl)c(Cl)c1
Mol. weight [g/mol]: 163.00
CAS: 95-77-2

Physical Properties

Property code	Value	Unit	Source
chs	-2748.60 ± 0.80	kJ/mol	NIST Webbook
gf	-76.06	kJ/mol	Joback Method
hf	-150.30 ± 2.50	kJ/mol	NIST Webbook
hfs	-231.60 ± 1.10	kJ/mol	NIST Webbook
hfus	19.13	kJ/mol	Joback Method
hsub	81.30 ± 2.30	kJ/mol	NIST Webbook
hsub	89.80 ± 0.40	kJ/mol	NIST Webbook
hsub	81.30 ± 2.30	kJ/mol	NIST Webbook
hvap	70.80 ± 0.20	kJ/mol	NIST Webbook
log10ws	-1.25		Estimated Solubility Method
log10ws	-1.25		Aqueous Solubility Prediction Method
logp	2.699		Crippen Method
mcvol	101.990	ml/mol	McGowan Method
pc	5080.25	kPa	Joback Method
rinpol	1374.00		NIST Webbook
rinpol	1430.00		NIST Webbook
rinpol	1387.00		NIST Webbook
rinpol	1385.00		NIST Webbook
rinpol	1408.00		NIST Webbook
rinpol	1378.00		NIST Webbook
rinpol	1430.00		NIST Webbook
rinpol	1385.00		NIST Webbook
rinpol	1429.40		NIST Webbook
rinpol	1382.00		NIST Webbook
rinpol	1383.00		NIST Webbook

rinpol	1391.00		NIST Webbook
rinpol	1378.00		NIST Webbook
rinpol	1391.00		NIST Webbook
rinpol	1384.00		NIST Webbook
ripol	2731.00		NIST Webbook
ripol	2777.00		NIST Webbook
ripol	2774.00		NIST Webbook
ripol	2731.00		NIST Webbook
ripol	2767.00		NIST Webbook
ripol	2774.00		NIST Webbook
ripol	2731.00		NIST Webbook
ripol	2752.00		NIST Webbook
ripol	2737.00		NIST Webbook
tb	418.70	K	NIST Webbook
tc	770.43	K	Joback Method
tf	341.00 ± 0.20	K	NIST Webbook
tf	338.11 ± 0.20	K	NIST Webbook
vc	0.328	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	193.91	J/mol×K	564.92	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	186.59	J/mol×K	523.82	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	20.93	kJ/mol	341.00	NIST Webbook
hfust	20.93	kJ/mol	341.00	NIST Webbook
hfust	20.93	kJ/mol	341.00	NIST Webbook
hvapt	66.70	kJ/mol	354.50	NIST Webbook

psub	2.70e-04	kPa	291.40	Thermochemistry of Chlorobenzenes and Chlorophenols: Ambient Temperature Vapor Pressures and Enthalpies of Phase Transitions	
psub	0.04	kPa	337.30	Thermochemistry of Chlorobenzenes and Chlorophenols: Ambient Temperature Vapor Pressures and Enthalpies of Phase Transitions	
psub	0.03	kPa	335.30	Thermochemistry of Chlorobenzenes and Chlorophenols: Ambient Temperature Vapor Pressures and Enthalpies of Phase Transitions	
psub	0.03	kPa	332.30	Thermochemistry of Chlorobenzenes and Chlorophenols: Ambient Temperature Vapor Pressures and Enthalpies of Phase Transitions	
psub	0.02	kPa	329.30	Thermochemistry of Chlorobenzenes and Chlorophenols: Ambient Temperature Vapor Pressures and Enthalpies of Phase Transitions	

psub	0.01	kPa	326.30	Thermochemistry of Chlorobenzenes and Chlorophenols: Ambient Temperature Vapor Pressures and Enthalpies of Phase Transitions	
psub	0.01	kPa	323.30	Thermochemistry of Chlorobenzenes and Chlorophenols: Ambient Temperature Vapor Pressures and Enthalpies of Phase Transitions	
psub	8.06e-03	kPa	320.40	Thermochemistry of Chlorobenzenes and Chlorophenols: Ambient Temperature Vapor Pressures and Enthalpies of Phase Transitions	
psub	5.87e-03	kPa	317.20	Thermochemistry of Chlorobenzenes and Chlorophenols: Ambient Temperature Vapor Pressures and Enthalpies of Phase Transitions	
psub	4.23e-03	kPa	314.30	Thermochemistry of Chlorobenzenes and Chlorophenols: Ambient Temperature Vapor Pressures and Enthalpies of Phase Transitions	

psub	2.47e-03	kPa	309.50	Thermochemistry of Chlorobenzenes and Chlorophenols: Ambient Temperature Vapor Pressures and Enthalpies of Phase Transitions
psub	1.77e-03	kPa	306.70	Thermochemistry of Chlorobenzenes and Chlorophenols: Ambient Temperature Vapor Pressures and Enthalpies of Phase Transitions
psub	1.21e-03	kPa	303.50	Thermochemistry of Chlorobenzenes and Chlorophenols: Ambient Temperature Vapor Pressures and Enthalpies of Phase Transitions
psub	8.60e-04	kPa	300.30	Thermochemistry of Chlorobenzenes and Chlorophenols: Ambient Temperature Vapor Pressures and Enthalpies of Phase Transitions
psub	4.00e-04	kPa	294.30	Thermochemistry of Chlorobenzenes and Chlorophenols: Ambient Temperature Vapor Pressures and Enthalpies of Phase Transitions
sfust	61.37	J/mol×K	341.00	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	526.70	K	102.00	NIST Webbook

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C95772&Units=SI

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
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