2,3-DICHLOROPHENOL

Other names: phenol, 2,3-dichloro-
Inchi: InChI=1S/C6H4Cl2O/c7-4-2-1-3-5(9)6(4)8/h1-3,9H
InchiKey: UMPSXRYVXUPCOS-UHFFFAOYSA-N
Formula: C6H4Cl2O
SMILES: Oc1cccc(Cl)c1Cl
Mol. weight [g/mol]: 163.00

Physical Properties

Property code	Value	Unit	Source
af	0.4941		Cheméo Relay (1.0)
chs	-2756.88	kJ/mol	NIST Webbook
gf	-76.06	kJ/mol	Joback Method
hf	-151.60 ± 2.50	kJ/mol	NIST Webbook
hfs	-223.30 ± 1.10	kJ/mol	NIST Webbook
hfus	19.13	kJ/mol	Joback Method
hsub	76.90 ± 0.40	kJ/mol	NIST Webbook
hsub	71.70 ± 2.20	kJ/mol	NIST Webbook
hsub	71.70 ± 2.20	kJ/mol	NIST Webbook
hvap	57.30 ± 0.20	kJ/mol	NIST Webbook
ie	8.67	eV	Cheméo Relay (1.0)
log10ws	-1.30		Estimated Solubility Method
log10ws	-1.30		Aqueous Solubility Prediction Method
logp	2.699		Crippen Method
mcvol	101.990	ml/mol	McGowan Method
pc	5080.25	kPa	Joback Method
rinpol	1180.00		NIST Webbook
rinpol	1188.00		NIST Webbook
rinpol	1200.00		NIST Webbook
rinpol	1193.50		NIST Webbook
rinpol	1200.00		NIST Webbook
rinpol	1180.00		NIST Webbook
rinpol	1169.00		NIST Webbook
rinpol	1144.00		NIST Webbook
rinpol	1193.50		NIST Webbook
rinpol	1165.00		NIST Webbook
rinpol	1155.00		NIST Webbook

rinpol	1173.00		NIST Webbook
rinpol	1200.00		NIST Webbook
ripol	2160.00		NIST Webbook
ripol	2160.00		NIST Webbook
ripol	2143.00		NIST Webbook
ripol	2152.00		NIST Webbook
ripol	2131.00		NIST Webbook
ripol	2107.00		NIST Webbook
ripol	2117.00		NIST Webbook
tb	479.20	K	NIST Webbook
tc	793.51	K	Cheméo Relay (1.0)
tf	330.82	K	Aqueous Solubility Prediction Method
tf	330.00 ± 0.20	K	NIST Webbook
vc	0.354	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	221.90	J/mol×K	770.43	Joback Method
cpg	186.59	J/mol×K	523.82	Joback Method
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
dvisc	0.0000885	Pa×s	523.82	Joback Method
dvisc	0.0017868	Pa×s	367.88	Joback Method
dvisc	0.0009180	Pa×s	393.87	Joback Method
dvisc	0.0005122	Pa×s	419.86	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
hfust	21.36	kJ/mol	330.00	NIST Webbook
hfust	21.36	kJ/mol	330.00	NIST Webbook
hfust	21.36	kJ/mol	330.00	NIST Webbook

psub	0.02	kPa	303.20	Thermochemistry of Chlorobenzenes and Chlorophenols: Ambient Temperature Vapor Pressures and Enthalpies of Phase Transitions	
psub	0.01	kPa	300.20	Thermochemistry of Chlorobenzenes and Chlorophenols: Ambient Temperature Vapor Pressures and Enthalpies of Phase Transitions	
psub	0.03	kPa	306.20	Thermochemistry of Chlorobenzenes and Chlorophenols: Ambient Temperature Vapor Pressures and Enthalpies of Phase Transitions	
psub	0.04	kPa	309.20	Thermochemistry of Chlorobenzenes and Chlorophenols: Ambient Temperature Vapor Pressures and Enthalpies of Phase Transitions	
psub	0.05	kPa	312.20	Thermochemistry of Chlorobenzenes and Chlorophenols: Ambient Temperature Vapor Pressures and Enthalpies of Phase Transitions	

psub	0.06	kPa	315.20	Thermochemistry of Chlorobenzenes and Chlorophenols: Ambient Temperature Vapor Pressures and Enthalpies of Phase Transitions	
psub	0.08	kPa	318.10	Thermochemistry of Chlorobenzenes and Chlorophenols: Ambient Temperature Vapor Pressures and Enthalpies of Phase Transitions	
psub	0.11	kPa	321.20	Thermochemistry of Chlorobenzenes and Chlorophenols: Ambient Temperature Vapor Pressures and Enthalpies of Phase Transitions	
psub	0.14	kPa	324.30	Thermochemistry of Chlorobenzenes and Chlorophenols: Ambient Temperature Vapor Pressures and Enthalpies of Phase Transitions	
psub	0.18	kPa	327.30	Thermochemistry of Chlorobenzenes and Chlorophenols: Ambient Temperature Vapor Pressures and Enthalpies of Phase Transitions	

psub	0.01	kPa	297.30	Thermochemistry of Chlorobenzenes and Chlorophenols: Ambient Temperature Vapor Pressures and Enthalpies of Phase Transitions
psub	7.80e-03	kPa	294.30	Thermochemistry of Chlorobenzenes and Chlorophenols: Ambient Temperature Vapor Pressures and Enthalpies of Phase Transitions
sfust	64.74	J/mol×K	330.00	NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C576249&Units=SI
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
Cheméo Relay (1.0, beta):	
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
Cheméo Relay (1.0):	
Estimated Solubility Method:	http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt

Legend

af:	Acentric Factor
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
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
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
sfust:	Entropy of fusion at a given temperature
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume