Phenol, 3,5-dichloro-

Other names: 3,5-Dichlorophenol
Inchi: InChI=1S/C6H4Cl2O/c7-4-1-5(8)3-6(9)2-4/h1-3,9H
InchiKey: VPOMSPZBQMDLTM-UHFFFAOYSA-N
Formula: C6H4Cl2O
SMILES: Oc1cc(Cl)cc(Cl)c1
Mol. weight [g/mol]: 163.00
CAS: 591-35-5

Physical Properties

Property code	Value	Unit	Source
chs	-2749.10 ± 0.60	kJ/mol	NIST Webbook
gf	-76.06	kJ/mol	Joback Method
hf	-148.20 ± 1.50	kJ/mol	NIST Webbook
hfs	-231.00 ± 1.00	kJ/mol	NIST Webbook
hfus	19.13	kJ/mol	Joback Method
hsub	82.80 ± 1.10	kJ/mol	NIST Webbook
hsub	82.80 ± 1.10	kJ/mol	NIST Webbook
hvap	53.67	kJ/mol	Joback Method
log10ws	-1.34		Estimated Solubility Method
log10ws	-1.34		Aqueous Solubility Prediction Method
logp	2.699		Crippen Method
mcvol	101.990	ml/mol	McGowan Method
pc	5080.25	kPa	Joback Method
rinpol	1367.00		NIST Webbook
rinpol	1362.00		NIST Webbook
rinpol	1362.00		NIST Webbook
rinpol	1399.90		NIST Webbook
rinpol	1391.00		NIST Webbook
rinpol	1400.00		NIST Webbook
rinpol	1395.00		NIST Webbook
rinpol	1392.00		NIST Webbook
rinpol	1391.00		NIST Webbook
rinpol	1370.00		NIST Webbook
rinpol	1375.00		NIST Webbook
rinpol	1358.00		NIST Webbook
rinpol	1375.00		NIST Webbook

rinpol	1370.00		NIST Webbook
rinpol	1391.00		NIST Webbook
ripol	2713.00		NIST Webbook
ripol	2707.00		NIST Webbook
ripol	2670.00		NIST Webbook
ripol	2675.00		NIST Webbook
ripol	2675.00		NIST Webbook
ripol	2691.00		NIST Webbook
ripol	2700.00		NIST Webbook
tb	506.20	K	NIST Webbook
tc	770.43	K	Joback Method
tf	340.48	K	Aqueous Solubility Prediction Method
tf	341.00 ± 0.20	K	NIST Webbook
vc	0.328	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	200.54	J/mol×K	606.02	Joback Method
cpg	221.90	J/mol×K	770.43	Joback Method
cpg	217.16	J/mol×K	729.33	Joback Method
cpg	212.08	J/mol×K	688.23	Joback Method
cpg	206.57	J/mol×K	647.12	Joback Method
cpg	186.59	J/mol×K	523.82	Joback Method
cpg	193.91	J/mol×K	564.92	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
dvisc	0.0017868	Pa×s	367.88	Joback Method
dvisc	0.0000885	Pa×s	523.82	Joback Method
hfust	20.51	kJ/mol	341.00	NIST Webbook
hfust	20.51	kJ/mol	341.00	NIST Webbook
hfust	20.51	kJ/mol	341.00	NIST Webbook
hsubt	71.80	kJ/mol	284.00	NIST Webbook
sfust	60.14	J/mol×K	341.00	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	396.20	K	1.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	2.24185e+01
Coeff. B	-8.93405e+03
Temperature range (K), min.	403.69
Temperature range (K), max.	522.25

Sources

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

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=C591355&Units=SI

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

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
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
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