Phenol, 2,4,6-trichloro-

Other names:	1,3,5-Trichloro-2-hydroxybenzene
	1,3,5-Trichlorophenol
	2,4,6 T
	2,4,6-Trichlorfenol
	2,4,6-Trichlorophenol
	Dowcide 2S
	Dowicide 2S
	NCI-C02904
	NSC 2165
	Omal
	Phenachlor
	Rcra waste number U231
	Trichloro-2-hydroxybenzene
Inchi:	InChI=1S/C6H3Cl3O/c7-3-1-4(8)6(10)5(9)2-3/h1-2,10H
InchiKey:	LINPIYWFGCPVIE-UHFFFAOYSA-N
Formula:	C6H3Cl3O
SMILES:	Oc1c(Cl)cc(Cl)cc1Cl
Mol. weight [g/mol]:	197.45
CAS:	88-06-2

Physical Properties

Property code	Value	Unit	Source
gf	-97.62	kJ/mol	Joback Method
hf	-178.11	kJ/mol	Joback Method
hfus	22.93	kJ/mol	Joback Method
hsub	82.30 ± 0.30	kJ/mol	NIST Webbook
hvap	67.20 ± 0.30	kJ/mol	NIST Webbook
hvap	66.10 ± 0.40	kJ/mol	NIST Webbook
log10ws	-2.34		Aqueous Solubility Prediction Method
log10ws	-2.34		Estimated Solubility Method
logp	3.352		Crippen Method
mcvol	114.230	ml/mol	McGowan Method
pc	4723.61	kPa	Joback Method
rinpol	1339.00		NIST Webbook
rinpol	1331.00		NIST Webbook

rinpol	1346.00	NIST Webbook
rinpol	1360.00	NIST Webbook
rinpol	1367.00	NIST Webbook
rinpol	1349.00	NIST Webbook
rinpol	1335.00	NIST Webbook
rinpol	1330.00	NIST Webbook
rinpol	1326.00	NIST Webbook
rinpol	1358.00	NIST Webbook
rinpol	1349.00	NIST Webbook
rinpol	1327.00	NIST Webbook
rinpol	1346.00	NIST Webbook
rinpol	1376.20	NIST Webbook
rinpol	1347.00	NIST Webbook
rinpol	1348.00	NIST Webbook
rinpol	1335.00	NIST Webbook
rinpol	1320.00	NIST Webbook
rinpol	1325.00	NIST Webbook
rinpol	1326.00	NIST Webbook
rinpol	1349.00	NIST Webbook
rinpol	1315.00	NIST Webbook
rinpol	1365.00	NIST Webbook
rinpol	1348.00	NIST Webbook
rinpol	1369.00	NIST Webbook
rinpol	1331.00	NIST Webbook
rinpol	1383.00	NIST Webbook
rinpol	1386.00	NIST Webbook
rinpol	1349.00	NIST Webbook
rinpol	231.00	NIST Webbook
rinpol	232.09	NIST Webbook
rinpol	266.23	NIST Webbook
rinpol	266.60	NIST Webbook
rinpol	1335.00	NIST Webbook
rinpol	1327.00	NIST Webbook
rinpol	1346.00	NIST Webbook
rinpol	1336.00	NIST Webbook
ripol	2306.00	NIST Webbook
ripol	2301.00	NIST Webbook
ripol	2270.00	NIST Webbook
ripol	2284.00	NIST Webbook
ripol	2301.00	NIST Webbook
ripol	2301.00	NIST Webbook
ripol	2343.02	NIST Webbook
ripol	2321.00	NIST Webbook
ripol	2344.63	NIST Webbook

ripol	2355.43		NIST Webbook
tb	519.20	K	NIST Webbook
tc	818.35	K	Joback Method
tf	340.90	K	Aqueous Solubility Prediction Method
vc	0.377	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	233.71	J/mol×K	818.35	Joback Method
cpg	209.69	J/mol×K	608.25	Joback Method
cpg	215.28	J/mol×K	650.27	Joback Method
cpg	220.38	J/mol×K	692.29	Joback Method
cpg	225.09	J/mol×K	734.31	Joback Method
cpg	229.51	J/mol×K	776.33	Joback Method
cpg	203.55	J/mol×K	566.23	Joback Method
dvisc	0.0000884	Pa×s	540.25	Joback Method
dvisc	0.0001265	Pa×s	514.26	Joback Method
dvisc	0.0001881	Pa×s	488.28	Joback Method
dvisc	0.0002925	Pa×s	462.29	Joback Method
dvisc	0.0004792	Pa×s	436.31	Joback Method
dvisc	0.0000638	Pa×s	566.23	Joback Method
dvisc	0.0008360	Pa×s	410.32	Joback Method
hvapt	58.80	kJ/mol	434.00	NIST Webbook
hvapt	62.50	kJ/mol	359.00	NIST Webbook
hvapt	58.20	kJ/mol	403.50	NIST Webbook
psub	5.93e-03	kPa	311.30	Thermochemistry of Chlorobenzenes and Chlorophenols: Ambient Temperature Vapor Pressures and Enthalpies of Phase Transitions

psub	0.01	kPa	317.30	Thermochemistry of Chlorobenzenes and Chlorophenols: Ambient Temperature Vapor Pressures and Enthalpies of Phase Transitions	
psub	0.01	kPa	320.30	Thermochemistry of Chlorobenzenes and Chlorophenols: Ambient Temperature Vapor Pressures and Enthalpies of Phase Transitions	
psub	0.02	kPa	323.30	Thermochemistry of Chlorobenzenes and Chlorophenols: Ambient Temperature Vapor Pressures and Enthalpies of Phase Transitions	
psub	0.03	kPa	326.30	Thermochemistry of Chlorobenzenes and Chlorophenols: Ambient Temperature Vapor Pressures and Enthalpies of Phase Transitions	
psub	0.03	kPa	329.40	Thermochemistry of Chlorobenzenes and Chlorophenols: Ambient Temperature Vapor Pressures and Enthalpies of Phase Transitions	

psub	0.05	kPa	332.50	Thermochemistry of Chlorobenzenes and Chlorophenols: Ambient Temperature Vapor Pressures and Enthalpies of Phase Transitions	
psub	0.06	kPa	335.50	Thermochemistry of Chlorobenzenes and Chlorophenols: Ambient Temperature Vapor Pressures and Enthalpies of Phase Transitions	
psub	0.08	kPa	338.20	Thermochemistry of Chlorobenzenes and Chlorophenols: Ambient Temperature Vapor Pressures and Enthalpies of Phase Transitions	
psub	0.09	kPa	340.30	Thermochemistry of Chlorobenzenes and Chlorophenols: Ambient Temperature Vapor Pressures and Enthalpies of Phase Transitions	
psub	3.19e-03	kPa	305.20	Thermochemistry of Chlorobenzenes and Chlorophenols: Ambient Temperature Vapor Pressures and Enthalpies of Phase Transitions	

psub	2.45e-03	kPa	302.30	Thermochemistry of Chlorobenzenes and Chlorophenols: Ambient Temperature Vapor Pressures and Enthalpies of Phase Transitions
psub	1.77e-03	kPa	299.40	Thermochemistry of Chlorobenzenes and Chlorophenols: Ambient Temperature Vapor Pressures and Enthalpies of Phase Transitions
psub	4.40e-03	kPa	308.30	Thermochemistry of Chlorobenzenes and Chlorophenols: Ambient Temperature Vapor Pressures and Enthalpies of Phase Transitions
psub	0.01	kPa	316.80	Thermochemistry of Chlorobenzenes and Chlorophenols: Ambient Temperature Vapor Pressures and Enthalpies of Phase Transitions
psub	8.05e-03	kPa	314.30	Thermochemistry of Chlorobenzenes and Chlorophenols: Ambient Temperature Vapor Pressures and Enthalpies of Phase Transitions

psub	0.01	kPa	316.80	Thermochemistry of Chlorobenzenes and Chlorophenols: Ambient Temperature Vapor Pressures and Enthalpies of Phase Transitions

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.41306e+01
Coeff. B	-4.96669e+03
Coeff. C	-3.43460e+01
Temperature range (K), min.	344.95
Temperature range (K), max.	597.52

Sources

Thermochemistry of Chlorobenzenes and Chlorophenols: Ambient Temperature Vapor Pressures and Enthalpies of Phase Transitions:	https://www.doi.org/10.1021/je060429r
Investigating the solubility of chlorophenols in hydrophobic ionic liquids:	https://www.doi.org/10.1016/j.jct.2019.03.026
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Estimated Solubility Method:	http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C88062&Units=SI

Legend

cpg:	Ideal gas heat capacity

dvisc:	Dynamic viscosity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume