Phenol, 2,4,5-trichloro-

Other names:	2,4,5-Trichlorophenol
	Collunosol
	Dowcide 2
	Dowicide 2
	NCI-C61187
	NSC 2266
	Nurelle
	Preventol I
	Rcra waste number U230
	TCP
Inchi:	InChI=1S/C6H3Cl3O/c7-3-1-5(9)6(10)2-4(3)8/h1-2,10H
InchiKey:	LHJGJYXLEPZJPM-UHFFFAOYSA-N
Formula:	C6H3Cl3O
SMILES:	Oc1cc(Cl)c(Cl)cc1Cl
Mol. weight [g/mol]:	197.45
CAS:	95-95-4

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
hvap	58.72	kJ/mol	Joback Method
log10ws	-2.21		Aqueous Solubility Prediction Method
log10ws	-2.21		Estimated Solubility Method
logp	3.352		Crippen Method
mcvol	114.230	ml/mol	McGowan Method
pc	4723.61	kPa	Joback Method
rinpol	1370.00		NIST Webbook
rinpol	1356.00		NIST Webbook
rinpol	1359.00		NIST Webbook
rinpol	1335.00		NIST Webbook
rinpol	1346.00		NIST Webbook
rinpol	1338.00		NIST Webbook
rinpol	1322.00		NIST Webbook

rinpol	1338.00		NIST Webbook
rinpol	1391.00		NIST Webbook
rinpol	1392.00		NIST Webbook
rinpol	1327.00		NIST Webbook
rinpol	1362.00		NIST Webbook
rinpol	1327.00		NIST Webbook
rinpol	1342.00		NIST Webbook
rinpol	1338.00		NIST Webbook
rinpol	1327.00		NIST Webbook
rinpol	1362.00		NIST Webbook
rinpol	1356.00		NIST Webbook
rinpol	1384.00		NIST Webbook
rinpol	1381.10		NIST Webbook
rinpol	231.90		NIST Webbook
rinpol	1355.00		NIST Webbook
ripol	2458.00		NIST Webbook
ripol	2420.00		NIST Webbook
ripol	2444.00		NIST Webbook
ripol	2458.00		NIST Webbook
ripol	2460.00		NIST Webbook
ripol	2453.00		NIST Webbook
ripol	2476.00		NIST Webbook
tb	566.23	K	Joback Method
tc	818.35	K	Joback Method
tf	341.20 ± 0.20	K	NIST Webbook
tf	339.00 ± 3.00	K	NIST Webbook
tf	342.00 ± 0.20	K	NIST Webbook
tf	340.85	K	Aqueous Solubility Prediction Method
vc	0.377	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	225.09	J/mol×K	734.31	Joback Method
cpg	233.71	J/mol×K	818.35	Joback Method
cpg	229.51	J/mol×K	776.33	Joback Method
cpg	203.55	J/mol×K	566.23	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

dvisc	0.0000638	Pa×s	566.23	Joback Method
dvisc	0.0001265	Pa×s	514.26	Joback Method
dvisc	0.0000884	Pa×s	540.25	Joback Method
dvisc	0.0008360	Pa×s	410.32	Joback Method
dvisc	0.0004792	Pa×s	436.31	Joback Method
dvisc	0.0002925	Pa×s	462.29	Joback Method
dvisc	0.0001881	Pa×s	488.28	Joback Method
hfust	21.59	kJ/mol	340.30	NIST Webbook
hfust	21.59	kJ/mol	340.30	NIST Webbook
hvapt	54.50	kJ/mol	435.00	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	521.20	K	98.70	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.36469e+01
Coeff. B	-4.70213e+03
Coeff. C	-3.56740e+01
Temperature range (K), min.	345.00
Temperature range (K), max.	599.79

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C95954&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

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

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
hfust:	Enthalpy of fusion at a given temperature
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
pvap:	Vapor pressure
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume