Phenol, 2,3,4,6-tetrachloro-

Other names:	1-Hydroxy-2,3,4,6-tetrachlorobenzene
	2,3,4,6-Tetrachlorophenol
	2,4,5,6-Tetrachlorophenol
	Dowicide 6
	TCP
Inchi:	InChI=1S/C6H2Cl4O/c7-2-1-3(8)6(11)5(10)4(2)9/h1,11H
InchiKey:	VGVRPFIJEJYOFN-UHFFFAOYSA-N
Formula:	C6H2Cl4O
SMILES:	Oc1c(Cl)cc(Cl)c(Cl)c1Cl
Mol. weight [g/mol]:	231.89
CAS:	58-90-2

Physical Properties

Property code	Value	Unit	Source
gf	-119.18	kJ/mol	Joback Method
hf	-205.32	kJ/mol	Joback Method
hfus	26.74	kJ/mol	Joback Method
hvap	63.77	kJ/mol	Joback Method
log10ws	-3.10		Aqueous Solubility Prediction Method
log10ws	-3.10		Estimated Solubility Method
logp	4.006		Crippen Method
mcvol	126.470	ml/mol	McGowan Method
pc	4403.25	kPa	Joback Method
rinpol	296.86		NIST Webbook
rinpol	264.80		NIST Webbook
rinpol	1519.00		NIST Webbook
rinpol	298.60		NIST Webbook
rinpol	1538.00		NIST Webbook
rinpol	1519.00		NIST Webbook
rinpol	1538.00		NIST Webbook
rinpol	1559.00		NIST Webbook
rinpol	1552.00		NIST Webbook
rinpol	1523.00		NIST Webbook
rinpol	1546.00		NIST Webbook
rinpol	1552.00		NIST Webbook

rinpol	1506.00		NIST Webbook
rinpol	1519.00		NIST Webbook
rinpol	1597.00		NIST Webbook
rinpol	1563.00		NIST Webbook
rinpol	264.80		NIST Webbook
rinpol	265.40		NIST Webbook
rinpol	1584.80		NIST Webbook
ripol	2620.00		NIST Webbook
ripol	2609.00		NIST Webbook
ripol	2602.00		NIST Webbook
ripol	2620.00		NIST Webbook
ripol	2615.00		NIST Webbook
ripol	2573.00		NIST Webbook
ripol	2554.00		NIST Webbook
ripol	2554.00		NIST Webbook
tb	608.64	K	Joback Method
tc	865.32	K	Joback Method
tf	341.00 ± 4.00	K	NIST Webbook
vc	0.425	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	218.56	J/mol×K	608.64	Joback Method
cpg	223.68	J/mol×K	651.42	Joback Method
cpg	228.36	J/mol×K	694.20	Joback Method
cpg	232.70	J/mol×K	736.98	Joback Method
cpg	236.77	J/mol×K	779.76	Joback Method
cpg	240.66	J/mol×K	822.54	Joback Method
cpg	244.46	J/mol×K	865.32	Joback Method
dvisc	0.0004365	Pa×s	452.76	Joback Method
dvisc	0.0002718	Pa×s	478.74	Joback Method
dvisc	0.0001777	Pa×s	504.72	Joback Method
dvisc	0.0001211	Pa×s	530.70	Joback Method
dvisc	0.0000855	Pa×s	556.68	Joback Method
dvisc	0.0000623	Pa×s	582.66	Joback Method
dvisc	0.0000467	Pa×s	608.64	Joback Method
hvapt	64.80	kJ/mol	460.50	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	423.20	K	2.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.34834e+01
Coeff. B	-5.03271e+03
Coeff. C	-3.70440e+01
Temperature range (K), min.	373.00
Temperature range (K), max.	652.90

Sources

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C58902&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

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