Ethane, pentachloro-

Other names:	1,1,1,2,2-pentachloroethane
	CHCl2CCl3
	ETHANEPENTACHLORIDE
	Ethane pentachloride
	Ethane, 1,1,1,2,2-pentachloro-
	NCI-C53894
	PENTALIN
	Pentachloorethaan
	Pentachloraethan
	Pentachlorethane
	Pentachloroethane
	Pentacloroetano
	Pentaline
	R-120
	Rcra waste number U184
	UN 1669
	freon 120
Inchi:	InChI=1S/C2HCl5/c3-1(4)2(5,6)7/h1H
InchiKey:	BNIXVQGCZULYKV-UHFFFAOYSA-N
Formula:	C2HCl5
SMILES:	ClC(Cl)C(Cl)(Cl)Cl
Mol. weight [g/mol]:	202.29
CAS:	76-01-7

Physical Properties

Property code	Value	Unit	Source
chl	-862.30 ± 8.40	kJ/mol	NIST Webbook
dm	1.00	debye	KDB
gf	-66.70	kJ/mol	KDB
hf	-142.40	kJ/mol	KDB
hf	-155.90 ± 4.30	kJ/mol	NIST Webbook
hf	-145.00	kJ/mol	NIST Webbook
hfl	-203.00 ± 4.00	kJ/mol	NIST Webbook
hfl	-191.00	kJ/mol	NIST Webbook
hfus	10.98	kJ/mol	Joback Method
hvap	47.40 ± 1.50	kJ/mol	NIST Webbook
ie	11.00	eV	NIST Webbook

ie	11.28	eV	NIST Webbook
log10ws	-2.60		Estimated Solubility Method
log10ws	-2.60		Aqueous Solubility Prediction Method
logp	3.160		Crippen Method
mcvol	100.240	ml/mol	McGowan Method
pc	3480.00	kPa	KDB
rinpol	965.00		NIST Webbook
rinpol	965.00		NIST Webbook
rinpol	951.00		NIST Webbook
rinpol	950.00		NIST Webbook
rinpol	953.00		NIST Webbook
rinpol	953.00		NIST Webbook
rinpol	953.00		NIST Webbook
rinpol	951.00		NIST Webbook
rinpol	957.00		NIST Webbook
rinpol	963.20		NIST Webbook
rinpol	965.00		NIST Webbook
rinpol	978.00		NIST Webbook
ripol	1454.62		NIST Webbook
ripol	1431.59		NIST Webbook
tb	435.10 ± 0.50	K	NIST Webbook
tb	435.00 ± 1.00	K	NIST Webbook
tb	435.20	K	NIST Webbook
tb	435.00	K	KDB
tb	434.65 ± 1.00	K	NIST Webbook
tc	646.00	K	KDB
tf	244.00	K	KDB
tf	243.50 ± 1.00	K	NIST Webbook
tf	244.22	K	Aqueous Solubility Prediction Method
vc	0.376	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	155.95	J/mol×K	658.19	Joback Method
cpg	137.11	J/mol×K	428.64	Joback Method
cpg	148.53	J/mol×K	543.42	Joback Method
cpg	151.39	J/mol×K	581.67	Joback Method
cpg	153.85	J/mol×K	619.93	Joback Method

cpg	145.23	J/mol×K	505.16	Joback Method
cpg	141.44	J/mol×K	466.90	Joback Method
cpl	196.20	J/mol×K	298.00	NIST Webbook
dvisc	0.0004728	Pa×s	428.64	Joback Method
dvisc	0.0008768	Pa×s	368.87	Joback Method
dvisc	0.0012956	Pa×s	338.98	Joback Method
dvisc	0.0020647	Pa×s	309.09	Joback Method
dvisc	0.0036356	Pa×s	279.21	Joback Method
dvisc	0.0006291	Pa×s	398.75	Joback Method
dvisc	0.0073315	Pa×s	249.32	Joback Method
hvapt	45.50	kJ/mol	366.50	NIST Webbook
hvapt	40.90	kJ/mol	354.00	NIST Webbook
hvapt	41.00	kJ/mol	433.50	KDB
rhol	1671.00	kg/m3	298.00	KDB
srf	0.03	N/m	298.20	KDB

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	342.20	K	4.90	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.37664e+01
Coeff. B	-3.40174e+03
Coeff. C	-6.33480e+01
Temperature range (K), min.	315.72
Temperature range (K), max.	465.68

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	1.06041e+02
Coeff. B	-9.09687e+03

Coeff. C	-1.35036e+01
Coeff. D	8.24216e-06
Temperature range (K), min.	244.15
Temperature range (K), max.	665.00

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
KDB:	https://www.cheric.org/files/research/kdb/mol/mol1552.mol
KDB Vapor Pressure Data:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1552
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C76017&Units=SI
Estimated Solubility Method:	http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt
Determination of Henry's Law Constants Using Internal Standards	https://www.doi.org/10.1021/je3010535
Aqueous Solubility Prediction Method with Benchmark Values:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa

Legend

chl:	Standard liquid enthalpy of combustion
cpg:	Ideal gas heat capacity
cpl:	Liquid phase heat capacity
dm:	Dipole Moment
dvisc:	Dynamic viscosity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfl:	Liquid phase 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
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
pvap:	Vapor pressure
rhol:	Liquid Density

rinpol:	Non-polar retention indices
ripol:	Polar retention indices
srf:	Surface Tension
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume