Ethane, 1,1,1,2-tetrachloro-

Other names:	1,1,1,2-Tetrachloroethane
	CH2ClCCl3
	NCI-C52459
	R-130a
	REFRIGERANT-130A
	Rcra waste number U208
	freon 130a
Inchi:	InChI=1S/C2H2Cl4/c3-1-2(4,5)6/h1H2
InchiKey:	QVLAWKAXOMEXPM-UHFFFAOYSA-N
Formula:	C2H2Cl4
SMILES:	ClCC(Cl)(Cl)Cl
Mol. weight [g/mol]:	167.85
CAS:	630-20-6

Physical Properties

Property code	Value	Unit	Source
chl	-973.90 ± 1.30	kJ/mol	NIST Webbook
gf	-78.92	kJ/mol	Joback Method
hf	-152.30 ± 2.40	kJ/mol	NIST Webbook
hf	-135.60	kJ/mol	NIST Webbook
hfl	-193.40 ± 2.30	kJ/mol	NIST Webbook
hfl	-178.00	kJ/mol	NIST Webbook
hfl	-193.50 ± 1.40	kJ/mol	NIST Webbook
hfus	10.31	kJ/mol	Joback Method
hvap	42.17	kJ/mol	NIST Webbook
hvap	45.70 ± 0.10	kJ/mol	NIST Webbook
hvap	41.10 ± 0.50	kJ/mol	NIST Webbook
ie	11.45	eV	NIST Webbook
ie	11.10	eV	NIST Webbook
log10ws	-2.18		Aqueous Solubility Prediction Method
log10ws	-2.18		Estimated Solubility Method
logp	2.595		Crippen Method
mcvol	88.000	ml/mol	McGowan Method
pc	4222.04	kPa	Joback Method
rinpol	843.00		NIST Webbook

rinpol	833.00		NIST Webbook
rinpol	837.00		NIST Webbook
rinpol	843.00		NIST Webbook
rinpol	843.00		NIST Webbook
rinpol	837.00		NIST Webbook
rinpol	835.00		NIST Webbook
rinpol	837.00		NIST Webbook
rinpol	827.20		NIST Webbook
rinpol	825.00		NIST Webbook
rinpol	821.50		NIST Webbook
rinpol	833.00		NIST Webbook
rinpol	850.00		NIST Webbook
rinpol	840.00		NIST Webbook
rinpol	869.00		NIST Webbook
rinpol	870.00		NIST Webbook
ripol	1255.00		NIST Webbook
ripol	1261.00		NIST Webbook
ripol	1255.00		NIST Webbook
ripol	1283.29		NIST Webbook
ripol	1267.53		NIST Webbook
ripol	1261.00		NIST Webbook
ripol	1276.65		NIST Webbook
tb	402.95 ± 0.20	K	NIST Webbook
tb	403.70	K	NIST Webbook
tb	411.20	K	NIST Webbook
tc	607.53	K	Joback Method
tf	203.08	K	Aqueous Solubility Prediction Method
vc	0.333	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	138.33	J/mol×K	571.55	Joback Method
cpg	140.97	J/mol×K	607.53	Joback Method
cpg	119.32	J/mol×K	391.65	Joback Method
cpg	124.00	J/mol×K	427.63	Joback Method
cpg	128.21	J/mol×K	463.61	Joback Method
cpg	131.98	J/mol×K	499.59	Joback Method
cpg	135.34	J/mol×K	535.57	Joback Method
dvisc	0.0005057	Pa×s	391.65	Joback Method

dvisc	0.0006564	Pa×s	365.44	Joback Method
dvisc	0.0058031	Pa×s	234.40	Joback Method
dvisc	0.0031493	Pa×s	260.61	Joback Method
dvisc	0.0019111	Pa×s	286.82	Joback Method
dvisc	0.0012609	Pa×s	313.02	Joback Method
dvisc	0.0008871	Pa×s	339.23	Joback Method
hvapt	39.20	kJ/mol	367.50	NIST Webbook
hvapt	40.10	kJ/mol	381.50	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.35773e+01
Coeff. B	-3.22872e+03
Coeff. C	-5.08100e+01
Temperature range (K), min.	293.76
Temperature range (K), max.	441.42

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	8.06625e+01
Coeff. B	-7.62320e+03
Coeff. C	-9.66669e+00
Coeff. D	5.22775e-06
Temperature range (K), min.	202.94
Temperature range (K), max.	624.00

Sources

KDB: https://www.cheric.org/files/research/kdb/mol/mol1559.mol

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C630206&Units=SI

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

KDB Vapor Pressure Data: https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1559

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

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
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Determination of Henry's Law Constants Using Internal Standards with Benchmark Values:	https://www.doi.org/10.1021/je3010535

Legend

chl:	Standard liquid 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
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
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