Ethane, 1,2-dichloro-1,1,2,2-tetrafluoro-

Other names: (CF2Cl)2
1,1,2,2-Tetrafluoro-1,2-Dichloroethane
1,2-DICHLORO-1,1,2,2-TETRAFLUOROETHANE
1,2-Dichlorotetrafluoroethane
Arcton 114
Arcton 33
CFC-114
Cryofluoran
Cryofluorane
Dichloro-1,1,2,2-tetrafluoroethane
Ethane, 1,2-dichlorotetrafluoro-
F 114
F 114 (halocarbon)
FC 114
FKW 114
FREON 114
Fluorane 114
Fluorocarbon 114
Frigen 114
Frigiderm
Genetron 114
Genetron 316
Halocarbon 114
Halon 242
Isotron 114
Ledon 114
Propellant 114
R 114
R 114 (halocarbon)
R-114
REFRIGERANT-114
Refrigerant 114
Refrigerant R114
Ucon 114
s-Dichlorotetrafluoroethane
sym-Dichlorotetrafluoroethane

Inchi: InChI=1S/C2Cl2F4/c3-1(5,6)2(4,7)8

InchiKey: DDMOUSALMHHKOS-UHFFFAOYSA-N

Formula: C2Cl2F4

SMILES: FC(F)(Cl)C(F)(F)Cl

Mol. weight [g/mol]: 170.92
CAS: 76-14-2

Physical Properties

Property code	Value	Unit	Source
af	0.2460		KDB
chl	-589.90 ± 6.80	kJ/mol	NIST Webbook
dm	0.50	debye	KDB
gf	-831.46	kJ/mol	Joback Method
hf	-898.50	kJ/mol	KDB
hf	-930.00 ± 10.00	kJ/mol	NIST Webbook
hf	-937.00 ± 7.30	kJ/mol	NIST Webbook
hfl	-960.20 ± 7.30	kJ/mol	NIST Webbook
hfus	6.82	kJ/mol	Joback Method
hvap	23.40 ± 0.42	kJ/mol	NIST Webbook
hvap	23.20 ± 0.40	kJ/mol	NIST Webbook
ie	12.85	eV	NIST Webbook
ie	12.47	eV	NIST Webbook
log10ws	-2.74		Estimated Solubility Method
log10ws	-3.12		Aqueous Solubility Prediction Method
logp	2.650		Crippen Method
mcvol	70.600	ml/mol	McGowan Method
pc	3393.00 ± 0.01	kPa	NIST Webbook
pc	3252.00	kPa	KDB
pc	3268.10	kPa	NIST Webbook
rhoc	581.82 ± 0.58	kg/m3	NIST Webbook
rinpol	359.00		NIST Webbook
rinpol	352.00		NIST Webbook
rinpol	352.00		NIST Webbook
rinpol	359.00		NIST Webbook
rinpol	361.00		NIST Webbook
sl	282.00	J/mol×K	NIST Webbook
tb	276.90	K	KDB
tb	277.30	K	NIST Webbook
tb	275.44 ± 0.20	K	NIST Webbook
tb	276.90	K	NIST Webbook
tb	276.70	K	NIST Webbook
tc	418.90 ± 0.33	K	NIST Webbook
tc	418.85 ± 0.04	K	NIST Webbook

tc	418.87	K	NIST Webbook
tc	418.78	K	KDB
tc	418.85 ± 0.30	K	NIST Webbook
tf	179.00	K	KDB
tt	179.00 ± 1.50	K	NIST Webbook
tt	180.62 ± 0.02	K	NIST Webbook
vc	0.297	m3/kmol	KDB
zc	0.2773860		KDB

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	135.13	J/mol×K	420.28	Joback Method
cpg	119.86	J/mol×K	338.05	Joback Method
cpg	125.42	J/mol×K	365.46	Joback Method
cpg	130.50	J/mol×K	392.87	Joback Method
cpg	143.11	J/mol×K	475.11	Joback Method
cpg	139.32	J/mol×K	447.70	Joback Method
cpg	113.79	J/mol×K	310.64	Joback Method
cpl	169.90	J/mol×K	293.30	NIST Webbook
cpl	169.90	J/mol×K	293.30	NIST Webbook
cpl	164.00	J/mol×K	298.15	NIST Webbook
hfust	1.51	kJ/mol	180.60	NIST Webbook
hvapt	25.30	kJ/mol	227.50	NIST Webbook
hvapt	25.10	kJ/mol	243.50	NIST Webbook
hvapt	24.30	kJ/mol	334.00	NIST Webbook
hvapt	23.26	kJ/mol	277.30	KDB
rhol	1480.00	kg/m3	277.00	KDB
srf	0.03	N/m	273.20	KDB

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.39608e+01
Coeff. B	-2.23751e+03
Coeff. C	-3.72400e+01

Temperature range (K), min.	180.63
Temperature range (K), max.	418.83

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	8.29995e+01
Coeff. B	-5.26528e+03
Coeff. C	-1.07600e+01
Coeff. D	1.49659e-05
Temperature range (K), min.	179.15
Temperature range (K), max.	418.85

Sources

Estimated Solubility Method: http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C76142&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

KDB: https://www.cheric.org/files/research/kdb/mol/mol1537.mol

Solubility Differences of Halocarbon Isomers in Ionic Liquid [emim][Tf2N]: https://www.doi.org/10.1021/je700295e

Joback Method: https://en.wikipedia.org/wiki/Joback_method

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

KDB Pure (Korean Thermophysical Properties Databank): https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1537

Aqueous Solubility Prediction Method: http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa

KDB Vapor Pressure Data: https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1537

Legend

af: Acentric Factor

chl: Standard liquid enthalpy of combustion

cpg: Ideal gas heat capacity

cpl: Liquid phase heat capacity

dm: Dipole Moment

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
hfust:	Enthalpy of fusion at a given temperature
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
rhoc:	Critical density
rhol:	Liquid Density
rinpol:	Non-polar retention indices
sl:	Liquid phase molar entropy at standard conditions
srf:	Surface Tension
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
tt:	Triple Point Temperature
vc:	Critical Volume
zc:	Critical Compressibility