Ethene, chlorotrifluoro-

Other names:	1,1,2-Trifluoro-2-chloroethylene
	1-Chloro-1,2,2-trifluoroethene
	1-Chloro-1,2,2-trifluoroethylene
	1-chloro-1,2,2-trifluroethene
	2-Chloro-1,1,2-trifluoroethylene
	C2F3Cl
	CHLOROTRIFLUOROETHENE
	CTFE
	Chlorotrifluoroethylene
	Chlortrifluoraethylen
	Daiflon
	Ethene, 1-chloro-1,2,2-trifluoro-
	Ethylene, chlorotrifluoro-
	Ethylene, trifluorochloro-
	Fluoroplast 3
	GENETRON 1113
	Monochlorotrifluoroethylene
	TRIFLUOROMONOCHLOROETHYLENE
	Trifluorchlorethylen
	Trifluorochloroethylene
	Trifluorovinyl Chloride
	Trithene
	UN 1082
	trifluorochloroethene
Inchi:	InChI=1S/C2ClF3/c3-1(4)2(5)6
InchiKey:	UUAGAQFQZIEFAH-UHFFFAOYSA-N
Formula:	C2ClF3
SMILES:	FC(F)=C(F)Cl
Mol. weight [g/mol]:	116.47
CAS:	79-38-9

Physical Properties

Property code	Value	Unit	Source
af	0.2520		KDB
chl	-816.00 ± 2.80	kJ/mol	NIST Webbook
dm	0.40	debye	KDB

gf	-567.28	kJ/mol	Joback Method
hf	-505.50 ± 4.70	kJ/mol	NIST Webbook
hf	-531.70	kJ/mol	KDB
hf	-527.00 ± 8.00	kJ/mol	NIST Webbook
hf	-510.00 ± 13.00	kJ/mol	NIST Webbook
hf	-564.80 ± 5.80	kJ/mol	NIST Webbook
hfl	-522.70 ± 4.70	kJ/mol	NIST Webbook
hfus	11.96	kJ/mol	Joback Method
hvap	17.20	kJ/mol	NIST Webbook
ie	9.82	eV	NIST Webbook
ie	9.84	eV	NIST Webbook
ie	10.26	eV	NIST Webbook
ie	9.76	eV	NIST Webbook
ie	10.60 ± 0.10	eV	NIST Webbook
ie	9.81 ± 0.03	eV	NIST Webbook
log10ws	-2.21		Crippen Method
logp	2.260		Crippen Method
mcvol	52.290	ml/mol	McGowan Method
pc	4050.00	kPa	KDB
rhoc	549.74 ± 30.28	kg/m3	NIST Webbook
rinpol	294.00		NIST Webbook
sl	220.66	J/mol×K	NIST Webbook
tb	244.80	K	NIST Webbook
tb	245.30	K	KDB
tb	246.00	K	NIST Webbook
tc	379.00	K	KDB
tf	118.30 ± 0.20	K	NIST Webbook
tf	115.00	K	KDB
tt	115.00 ± 0.05	K	NIST Webbook
vc	0.212	m3/kmol	KDB
zc	0.2724680		KDB

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	86.66	J/mol×K	388.95	Joback Method
cpg	83.76	J/mol×K	362.79	Joback Method
cpg	80.65	J/mol×K	336.63	Joback Method
cpg	77.34	J/mol×K	310.48	Joback Method
cpg	91.91	J/mol×K	441.26	Joback Method
cpg	89.38	J/mol×K	415.11	Joback Method

cpg	73.81	J/mol×K	284.32	Joback Method
cpl	122.42	J/mol×K	244.80	NIST Webbook
hfust	5.55	kJ/mol	115.00	NIST Webbook
hfust	5.55	kJ/mol	115.00	NIST Webbook
hfust	5.55	kJ/mol	115.00	NIST Webbook
hfust	5.28	kJ/mol	118.30	NIST Webbook
hvapt	21.90	kJ/mol	222.50	NIST Webbook
hvapt	21.70	kJ/mol	234.50	NIST Webbook
hvapt	20.20	kJ/mol	338.50	NIST Webbook
hvapt	21.80	kJ/mol	234.00	NIST Webbook
pvap	294.40	kPa	272.54	Vapor-Liquid Equilibria of the Perfluoromethyl Vinyl Ether and Chlorotrifluoroethylene System
pvap	248.00	kPa	267.67	Vapor-Liquid Equilibria of the Perfluoromethyl Vinyl Ether and Chlorotrifluoroethylene System
pvap	347.80	kPa	277.45	Vapor-Liquid Equilibria of the Perfluoromethyl Vinyl Ether and Chlorotrifluoroethylene System
pvap	408.10	kPa	282.62	Vapor-Liquid Equilibria of the Perfluoromethyl Vinyl Ether and Chlorotrifluoroethylene System
rhol	1305.00	kg/m3	293.00	KDB
sfust	44.60	J/mol×K	118.30	NIST Webbook
sfust	48.28	J/mol×K	115.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.41890e+01
Coeff. B	-2.02995e+03
Coeff. C	-3.26990e+01
Temperature range (K), min.	178.72
Temperature range (K), max.	379.15

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	9.72054e+01
Coeff. B	-5.06861e+03
Coeff. C	-1.33563e+01
Coeff. D	2.63215e-05
Temperature range (K), min.	115.00
Temperature range (K), max.	379.15

Sources

Vapor-Liquid Equilibria of the Perfluoromethyl Vinyl Ether and Chlorotrifluoroethylene System:	https://www.doi.org/10.1021/je7001144
KDB:	https://www.cheric.org/files/research/kdb/mol/mol1713.mol
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C79389&Units=SI
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
KDB Vapor Pressure Data:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1713
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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
sfust:	Entropy of fusion at a given temperature
sl:	Liquid phase molar entropy at standard conditions
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
tt:	Triple Point Temperature
vc:	Critical Volume
zc:	Critical Compressibility