Ethane, 1,1,2-trichloro-1,2,2-trifluoro-

Other names:

1,1,2-TRICHLORO-1,2,2-TRIFLUOROETHANE
1,1,2-Trichlorotrifluoroethane
1,1,2-Trifluoro-1,2,2-trichloroethane
1,1,2-Trifluorotrichloroethane
1,1,2-trichlorotrifluoroethane (Freon 113)
1,2,2-Trichlorotrifluoroethane
1,2,2-Trifluorotrichloroethane
ARCTON 63
Arklone
Arklone P
Asahifron 113
CFC-113
CFCl2CF2Cl
Daiflon S 3
Delifrene LS
Distillex DS5
F 113
FC 113
FC 133
Fluorocarbon 113
Forane 113
Freon 113
Freon 113 TR-T
Freon F113
Freon R 113
Freon TF
Freon TF (113)
Frigen 113
Frigen 113 TR
Frigen 113 TR-T
Frigen 113A
Genesolv D
Genetron 113
Halocarbon 113
Halon 113
Isceon 113
Kaiser chemicals 11
Khladon 113
LEDON 113
R 113

R 113(Halocarbon)
R-113
REFRIGERANT-113
Refrigerant 113
Refrigerant R 113
Trichloro 1,2,2-trifluoroethane

Inchi: InChI=1S/C2Cl3F3/c3-1(4,6)2(5,7)8
InchiKey: AJDIZQLSFPQPEY-UHFFFAOYSA-N
Formula: C2Cl3F3
SMILES: FC(F)(Cl)C(F)(Cl)Cl
Mol. weight [g/mol]: 187.38
CAS: 76-13-1

Physical Properties

Property code	Value	Unit	Source
chl	-641.60 ± 1.90	kJ/mol	NIST Webbook
gf	-648.58	kJ/mol	Joback Method
hf	-726.80 ± 4.30	kJ/mol	NIST Webbook
hfl	-755.00 ± 4.30	kJ/mol	NIST Webbook
hfus	7.94	kJ/mol	Joback Method
hvap	28.70	kJ/mol	NIST Webbook
hvap	28.20 ± 0.40	kJ/mol	NIST Webbook
hvap	28.20 ± 0.40	kJ/mol	NIST Webbook
hvap	28.61	kJ/mol	NIST Webbook
hvap	28.40 ± 0.10	kJ/mol	NIST Webbook
ie	11.99 ± 0.02	eV	NIST Webbook
ie	12.05	eV	NIST Webbook
log10ws	-3.04		Estimated Solubility Method
log10ws	-3.04		Aqueous Solubility Prediction Method
logp	2.919		Crippen Method
mcvol	81.070	ml/mol	McGowan Method
pc	3420.00	kPa	KDB
pc	3412.89	kPa	NIST Webbook
pc	3410.82 ± 6.89	kPa	NIST Webbook
pc	3379.00 ± 5.00	kPa	NIST Webbook
rhoc	569.92 ± 9.61	kg/m3	NIST Webbook
rhoc	575.24 ± 1.87	kg/m3	NIST Webbook
rhoc	569.62 ± 5.70	kg/m3	NIST Webbook
rinpol	540.00		NIST Webbook

rinpol	530.00		NIST Webbook
rinpol	530.00		NIST Webbook
rinpol	555.00		NIST Webbook
rinpol	527.00		NIST Webbook
rinpol	522.00		NIST Webbook
rinpol	522.00		NIST Webbook
rinpol	526.00		NIST Webbook
rinpol	532.00		NIST Webbook
rinpol	524.00		NIST Webbook
rinpol	528.00		NIST Webbook
ripol	660.00		NIST Webbook
ripol	660.00		NIST Webbook
sl	289.50	J/mol×K	NIST Webbook
tb	320.70	K	NIST Webbook
tb	321.00	K	NIST Webbook
tb	320.70	K	NIST Webbook
tb	320.80	K	KDB
tb	320.90	K	NIST Webbook
tb	320.42 ± 0.10	K	NIST Webbook
tc	487.30	K	KDB
tf	238.00	K	KDB
tf	238.15	K	NIST Webbook
tt	236.92 ± 0.02	K	NIST Webbook
tt	236.55 ± 0.10	K	NIST Webbook
tt	237.93 ± 0.02	K	NIST Webbook
vc	0.325	m3/kmol	KDB
zc	0.2743320		KDB

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	142.49	J/mol×K	441.33	Joback Method
cpg	132.62	J/mol×K	379.64	Joback Method
cpg	126.81	J/mol×K	348.80	Joback Method
cpg	146.63	J/mol×K	472.18	Joback Method
cpg	150.28	J/mol×K	503.02	Joback Method
cpg	153.48	J/mol×K	533.87	Joback Method
cpg	137.83	J/mol×K	410.49	Joback Method
cpl	172.80	J/mol×K	298.15	NIST Webbook
cpl	179.80	J/mol×K	298.15	NIST Webbook
cpl	172.50	J/mol×K	303.15	NIST Webbook

cpl	177.00	J/mol×K	298.20	NIST Webbook
cpl	177.00	J/mol×K	298.20	NIST Webbook
cpl	172.90	J/mol×K	298.15	NIST Webbook
hfust	2.33	kJ/mol	273.93	NIST Webbook
hfust	2.47	kJ/mol	236.90	NIST Webbook
hfust	0.83	kJ/mol	82.50	NIST Webbook
hfust	2.47	kJ/mol	236.90	NIST Webbook
hsubt	32.90	kJ/mol	219.00	NIST Webbook
hvapt	27.50 ± 0.10	kJ/mol	313.00	NIST Webbook
hvapt	28.30	kJ/mol	296.00	NIST Webbook
hvapt	30.80	kJ/mol	302.00	NIST Webbook
hvapt	28.20	kJ/mol	295.50	NIST Webbook
hvapt	26.60 ± 0.10	kJ/mol	328.00	NIST Webbook
hvapt	27.04	kJ/mol	320.70	NIST Webbook
hvapt	28.80	kJ/mol	307.00	NIST Webbook
hvapt	26.90	kJ/mol	416.50	NIST Webbook
hvapt	30.90	kJ/mol	301.00	NIST Webbook
sfust	8.49	J/mol×K	273.93	NIST Webbook
sfust	10.08	J/mol×K	82.50	NIST Webbook
sfust	10.42	J/mol×K	236.90	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.40069e+01
Coeff. B	-2.62436e+03
Coeff. C	-4.14730e+01
Temperature range (K), min.	232.76
Temperature range (K), max.	487.21

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	1.11463e+02
Coeff. B	-7.08030e+03
Coeff. C	-1.49859e+01
Coeff. D	1.67919e-05
Temperature range (K), min.	238.15

Temperature range (K), max.	487.25

Sources

Hydrogen substitution effect on the solubility of perhalogenated compounds in ionic liquid [bmim][PF6]:	https://www.doi.org/10.1016/j.fluid.2007.07.035
Determination of Henry's Law Constants Using Internal Standards with Benchmark Values:	https://www.doi.org/10.1021/je3010535
KDB Pure (Korean Thermophysical Properties Databank):	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1539
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
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=C76131&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
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=1539
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Solubility Differences of Halocarbon Isomers in Ionic Liquid [emim][Tf2N]:	https://www.doi.org/10.1021/je700295e
KDB:	https://www.cheric.org/files/research/kdb/mol/mol1539.mol

Legend

chl:	Standard liquid enthalpy of combustion
cpg:	Ideal gas heat capacity
cpl:	Liquid phase heat capacity
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
hsubt:	Enthalpy of sublimation 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

rinpol:	Non-polar retention indices
ripol:	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