Trichloromonofluoromethane

Other names:

ARCTON 9
Algofrene Type 1
Arcton 11
CCl3F
CFCl3
Chladone 11
Chlorofluoromethane (CCl3F)
Daiflon 11
Daiflon S 1
Distillex DS6
Dymel 11
Electro-CF 11
F 11
F 11 (halocarbon)
F 11B
FC 11
FC 11, Halocarbon
FKW 11
Fluon 11
Fluorocarbon 11
Fluorochloroform
Fluorotrichloromethane
Freon 11
Freon 11A
Freon MF
Frigen 11
Frigen 11A
Frigen S 11
Genetron 11
Genetron 11SBA
Halon 11
Isceon 131
Isotron 11
Kaltron 11
Khladon 11
Ledon 11
Methane, fluorotrichloro-
Methane, trichlorofluoro-
Monofluorotrichloromethane
Propellant 11

	R 11
	R 11, Halocarbon
	R-11
	REFRIGERANT-11
	Refrigerant 11
	Refrigerant R11
	Trichlorofluorocarbon
	Trichlorofluoromethane
	Trichloromethyl fluoride
	Tricloroflurmethane
Inchi:	InChI=1S/CCl3F/c2-1(3,4)5
InchiKey:	CYRMSUTZVYGINF-UHFFFAOYSA-N
Formula:	CCl3F
SMILES:	FC(Cl)(Cl)Cl
Mol. weight [g/mol]:	137.37
CAS:	75-69-4

Physical Properties

Property code	Value	Unit	Source
af	0.1890		KDB
dm	0.50	debye	KDB
ea	1.10 ± 0.30	eV	NIST Webbook
ea	1.02	eV	NIST Webbook
gf	-245.50	kJ/mol	KDB
hf	-268.30 ± 8.40	kJ/mol	NIST Webbook
hf	-284.70	kJ/mol	KDB
hf	-290.00 ± 20.00	kJ/mol	NIST Webbook
hf	-278.00 ± 8.80	kJ/mol	NIST Webbook
hfus	6.60	kJ/mol	Joback Method
hvap	28.86	kJ/mol	Joback Method
ie	11.73 ± 0.02	eV	NIST Webbook
ie	11.46 ± 0.02	eV	NIST Webbook
ie	11.68 ± 0.13	eV	NIST Webbook
ie	11.76 ± 0.01	eV	NIST Webbook
ie	11.90	eV	NIST Webbook
ie	11.77 ± 0.02	eV	NIST Webbook
ie	11.77 ± 0.01	eV	NIST Webbook
ie	11.85	eV	NIST Webbook
log10ws	-2.15		Crippen Method
logp	2.284		Crippen Method

mcvol	63.440	ml/mol	McGowan Method
pc	4370.00 ± 50.00	kPa	NIST Webbook
pc	4405.73	kPa	NIST Webbook
pc	4410.00	kPa	KDB
pc	4466.00 ± 12.00	kPa	NIST Webbook
rhoc	570.21 ± 0.55	kg/m3	NIST Webbook
rhoc	553.59 ± 1.37	kg/m3	NIST Webbook
rhoc	553.59 ± 5.54	kg/m3	NIST Webbook
rinpol	482.00		NIST Webbook
rinpol	470.00		NIST Webbook
rinpol	484.00		NIST Webbook
rinpol	460.00		NIST Webbook
rinpol	486.00		NIST Webbook
rinpol	484.00		NIST Webbook
rinpol	482.00		NIST Webbook
rinpol	484.00		NIST Webbook
rinpol	460.00		NIST Webbook
rinpol	478.00		NIST Webbook
rinpol	478.00		NIST Webbook
rinpol	486.00		NIST Webbook
rinpol	470.00		NIST Webbook
rinpol	485.00		NIST Webbook
ripol	605.00		NIST Webbook
ripol	605.00		NIST Webbook
sl	225.60	J/mol×K	NIST Webbook
tb	296.92	K	NIST Webbook
tb	296.90	K	NIST Webbook
tb	296.90	K	KDB
tb	296.80 ± 0.05	K	NIST Webbook
tc	471.10 ± 0.50	K	NIST Webbook
tc	471.15 ± 0.10	K	NIST Webbook
tc	471.20	K	KDB
tc	471.15 ± 0.40	K	NIST Webbook
tc	471.15	K	NIST Webbook
tc	471.15 ± 0.04	K	NIST Webbook
tf	162.70 ± 0.10	K	NIST Webbook
tf	165.40 ± 0.20	K	NIST Webbook
tf	162.67 ± 0.05	K	NIST Webbook
tf	162.04	K	KDB
tf	162.00 ± 2.00	K	NIST Webbook
tf	162.72 ± 0.01	K	NIST Webbook
tt	162.19 ± 0.05	K	NIST Webbook
tt	162.70 ± 0.01	K	NIST Webbook
tt	162.10 ± 0.20	K	NIST Webbook

tt	162.68 ± 0.07	K	NIST Webbook
tt	162.69 ± 0.06	K	NIST Webbook
tt	162.67 ± 0.06	K	NIST Webbook
tt	162.68 ± 0.03	K	NIST Webbook
tt	162.65 ± 0.02	K	NIST Webbook
tt	162.69 ± 0.03	K	NIST Webbook
vc	0.248	m3/kmol	KDB
vc	0.247 ± 0.006	m3/kmol	NIST Webbook
zc	0.2791570		KDB
zra	0.27		KDB

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	93.42	J/mol×K	493.01	Joback Method
cpg	91.42	J/mol×K	460.53	Joback Method
cpg	89.14	J/mol×K	428.05	Joback Method
cpg	86.55	J/mol×K	395.57	Joback Method
cpg	83.63	J/mol×K	363.09	Joback Method
cpg	95.16	J/mol×K	525.49	Joback Method
cpg	80.37	J/mol×K	330.61	Joback Method
cpl	126.70	J/mol×K	298.15	NIST Webbook
cpl	121.55	J/mol×K	298.15	NIST Webbook
cpl	122.50	J/mol×K	303.15	NIST Webbook
hfust	6.90	kJ/mol	162.70	NIST Webbook
hfust	7.90	kJ/mol	165.40	NIST Webbook
hfust	6.89	kJ/mol	162.68	NIST Webbook
hvapt	25.60	kJ/mol	329.00	NIST Webbook
hvapt	25.20	kJ/mol	290.00	NIST Webbook
hvapt	24.77	kJ/mol	297.10	KDB
hvapt	25.21	kJ/mol	290.40	NIST Webbook
hvapt	28.50	kJ/mol	257.00	NIST Webbook
hvapt	28.20	kJ/mol	231.00	NIST Webbook
hvapt	27.10	kJ/mol	265.00	NIST Webbook
hvapt	27.30	kJ/mol	265.00	NIST Webbook
hvapt	25.10	kJ/mol	446.00	NIST Webbook
hvapt	24.70	kJ/mol	393.00	NIST Webbook
hvapt	26.40	kJ/mol	289.00	NIST Webbook
rhol	1494.00	kg/m3	290.00	KDB
sfust	47.80	J/mol×K	165.40	NIST Webbook
sfust	42.38	J/mol×K	162.68	NIST Webbook

srf	0.02	N/m	277.60	KDB
svapt	86.81	J/mol×K	290.40	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.40921e+01
Coeff. B	-2.49136e+03
Coeff. C	-3.38850e+01
Temperature range (K), min.	214.36
Temperature range (K), max.	471.11

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	7.72409e+01
Coeff. B	-5.39795e+03
Coeff. C	-9.73971e+00
Coeff. D	1.15758e-05
Temperature range (K), min.	162.04
Temperature range (K), max.	471.20

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

KDB Vapor Pressure Data: https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1507

KDB: https://www.cheric.org/files/research/kdb/mol/mol1507.mol

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

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

Determination of Henry's Law Constants Using Internal Standards With Benchmark Values: https://www.doi.org/10.1021/je3010535

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C75694&Units=SI

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

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

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

Legend

af:	Acentric Factor
cpg:	Ideal gas heat capacity
cpl:	Liquid phase heat capacity
dm:	Dipole Moment
ea:	Electron affinity
gf:	Standard Gibbs free energy of formation
hf:	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
ripol:	Polar retention indices
sfust:	Entropy of fusion at a given temperature
sl:	Liquid phase molar entropy at standard conditions
srf:	Surface Tension
svapt:	Entropy of vaporization at a given temperature
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
tt:	Triple Point Temperature
vc:	Critical Volume
zc:	Critical Compressibility
zra:	Rackett Parameter