Chlorotrifluoromethane

Other names:	Arcton 3
	CClF3
	CF3Cl
	CFC-13
	Chlorotrifluromethane
	F 13
	FC 13
	Freon 13
	Frigen 13
	Genetron 13
	Halocarbon 13
	Halocarbon 13/ucon 13
	Khladon 13
	Methane, chlorotrifluoro-
	Monochlorotrifluoromethane
	R 13
	Refrigerant 13
	Trifluorochloromethane
	Trifluoromethyl chloride
	Trifluoromonochlorocarbon
	UN 1022
Inchi:	InChI=1S/CClF3/c2-1(3,4)5
InchiKey:	AFYPFACVUDMOHA-UHFFFAOYSA-N
Formula:	CClF3
SMILES:	FC(F)(F)Cl
Mol. weight [g/mol]:	104.46
CAS:	75-72-9

Physical Properties

Property code	Value	Unit	Source
affp	571.30	kJ/mol	NIST Webbook
basg	541.50	kJ/mol	NIST Webbook
gf	-635.98	kJ/mol	Joback Method
hf	-695.40 ± 9.20	kJ/mol	NIST Webbook
hf	-699.00	kJ/mol	NIST Webbook
hf	-715.00 ± 4.00	kJ/mol	NIST Webbook

hf	-708.80 ± 4.20	kJ/mol	NIST Webbook
hf	-705.00 ± 3.40	kJ/mol	NIST Webbook
hf	-739.50 ± 5.00	kJ/mol	NIST Webbook
hfus	4.37	kJ/mol	Joback Method
hvap	18.46	kJ/mol	Joback Method
ie	12.39	eV	NIST Webbook
ie	12.60 ± 0.02	eV	NIST Webbook
ie	13.08 ± 0.02	eV	NIST Webbook
ie	13.08 ± 0.02	eV	NIST Webbook
ie	13.00	eV	NIST Webbook
ie	13.10	eV	NIST Webbook
ie	13.08 ± 0.01	eV	NIST Webbook
ie	12.91 ± 0.03	eV	NIST Webbook
ie	12.39	eV	NIST Webbook
ie	12.45	eV	NIST Webbook
ie	13.00 ± 1.00	eV	NIST Webbook
ie	12.60 ± 0.40	eV	NIST Webbook
log10ws	-1.55		Crippen Method
logp	1.745		Crippen Method
mcvol	42.500	ml/mol	McGowan Method
pc	3885.00 ± 6.00	kPa	NIST Webbook
pc	3868.00 ± 10.00	kPa	NIST Webbook
pc	3867.94	kPa	NIST Webbook
pc	3879.00 ± 9.80	kPa	NIST Webbook
rhoc	582.36 ± 3.13	kg/m3	NIST Webbook
rhoc	598.86 ± 0.52	kg/m3	NIST Webbook
rhoc	579.75	kg/m3	NIST Webbook
rhoc	577.66 ± 3.13	kg/m3	NIST Webbook
rinpol	190.00		NIST Webbook
rinpol	209.00		NIST Webbook
rinpol	209.00		NIST Webbook
rinpol	190.00		NIST Webbook
tb	191.80 ± 0.30	K	NIST Webbook
tb	191.80 ± 0.30	K	NIST Webbook
tb	191.65 ± 0.05	K	NIST Webbook
tb	191.70	K	NIST Webbook
tc	301.90 ± 0.10	K	NIST Webbook
tc	301.98	K	NIST Webbook
tc	301.88 ± 0.05	K	NIST Webbook
tc	301.92 ± 0.08	K	NIST Webbook
tc	301.80	K	NIST Webbook
tc	301.54 ± 0.20	K	NIST Webbook
tc	301.92 ± 0.30	K	NIST Webbook
tf	92.20 ± 0.30	K	NIST Webbook

tf	92.03	K	NIST Webbook
tt	92.00 ± 2.00	K	NIST Webbook
vc	0.183	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	78.50	J/mol×K	403.52	Joback Method
cpg	64.09	J/mol×K	279.16	Joback Method
cpg	67.41	J/mol×K	304.03	Joback Method
cpg	70.50	J/mol×K	328.90	Joback Method
cpg	73.37	J/mol×K	353.78	Joback Method
cpg	76.04	J/mol×K	378.65	Joback Method
cpg	60.54	J/mol×K	254.29	Joback Method
hvapt	16.00	kJ/mol	285.00	NIST Webbook
hvapt	17.00	kJ/mol	159.00	NIST Webbook
hvapt	15.70	kJ/mol	215.00	NIST Webbook
hvapt	15.70	kJ/mol	257.00	NIST Webbook
hvapt	16.80	kJ/mol	168.50	NIST Webbook
hvapt	17.10	kJ/mol	157.50	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	4.10990e+01
Coeff. B	-2.65987e+03
Coeff. C	-4.37378e+00
Coeff. D	1.02412e-05
Temperature range (K), min.	92.15
Temperature range (K), max.	302.00

Sources

KDB:	https://www.cheric.org/files/research/kdb/mol/mol1505.mol
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C75729&Units=SI
KDB Pure (Korean Thermophysical Properties Databank):	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1505
KDB Vapor Pressure Data:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1505
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

affp:	Proton affinity
basg:	Gas basicity
cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	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
rhoc:	Critical density
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
tt:	Triple Point Temperature
vc:	Critical Volume