Pentafluoroethyl chloride

Other names:	1-Chloro-1,1,2,2,2-pentafluoroethane
	1-Chloropentafluoroethane
	CF3CF2Cl
	CFC 115
	Chloropentafluoroethane
	Chloroperfluoroethane
	Ethane, 1-chloro-1,1,2,2,2-pentafluoro-
	Ethane, chloropentafluoro-
	F-115
	FC 115
	FKW 115
	FLUOROCARBON 115
	FREON 115
	Genetron 115
	Monochloropentafluoroethane
	Pentafluorochloroethane
	Perfluoroethyl chloride
	Propellant 115
	R 115
	R-115
	REFRIGERANT-115
Inchi:	InChI=1S/C2ClF5/c3-1(4,5)2(6,7)8
InchiKey:	RFCAUADVODFSLZ-UHFFFAOYSA-N
Formula:	C2ClF5
SMILES:	FC(F)(F)C(F)(F)Cl
Mol. weight [g/mol]:	154.47
CAS:	76-15-3

Physical Properties

Property code	Value	Unit	Source
af	0.2790		KDB
dm	0.30	debye	KDB
gf	-1014.34	kJ/mol	Joback Method
hf	-1114.00 ± 10.00	kJ/mol	NIST Webbook
hfus	5.70	kJ/mol	Joback Method
hvap	17.75	kJ/mol	Joback Method

ie	12.96	eV	NIST Webbook
ie	12.60	eV	NIST Webbook
log10ws	-2.28		Crippen Method
logp	2.380		Crippen Method
mcvol	60.130	ml/mol	McGowan Method
pc	3157.29 ± 7.09	kPa	NIST Webbook
pc	3120.00 ± 8.00	kPa	NIST Webbook
pc	3229.00	kPa	KDB
rhoc	603.96 ± 4.63	kg/m3	NIST Webbook
rhoc	613.08 ± 1.50	kg/m3	NIST Webbook
rinpol	270.00		NIST Webbook
sl	248.03	J/mol×K	NIST Webbook
tb	235.50 ± 0.50	K	NIST Webbook
tb	235.20	K	NIST Webbook
tb	263.00 ± 3.00	K	NIST Webbook
tb	235.20	K	KDB
tb	235.00 ± 3.00	K	NIST Webbook
tc	353.20	K	KDB
tc	352.94 ± 0.05	K	NIST Webbook
tc	353.10 ± 0.15	K	NIST Webbook
tf	173.71	K	KDB
tt	173.71	K	KDB
tt	173.71 ± 0.05	K	NIST Webbook
vc	0.252	m3/kmol	KDB
zc	0.2770840		KDB

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	126.00	J/mol×K	392.44	Joback Method
cpg	99.25	J/mol×K	272.48	Joback Method
cpg	105.39	J/mol×K	296.47	Joback Method
cpg	111.12	J/mol×K	320.46	Joback Method
cpg	116.46	J/mol×K	344.46	Joback Method
cpg	121.41	J/mol×K	368.45	Joback Method
cpg	130.23	J/mol×K	416.43	Joback Method
cpl	145.27	J/mol×K	234.04	NIST Webbook
hfust	1.88	kJ/mol	173.70	NIST Webbook
hfust	2.63	kJ/mol	80.24	NIST Webbook
hfust	1.88	kJ/mol	173.70	NIST Webbook
hvapt	20.10	kJ/mol	249.50	NIST Webbook

hvapt	19.70	kJ/mol	289.50	NIST Webbook
hvapt	19.41	kJ/mol	234.04	NIST Webbook
hvapt	19.46	kJ/mol	234.70	KDB
hvapt	19.70	kJ/mol	332.50	NIST Webbook
hvapt	20.90	kJ/mol	206.00	NIST Webbook
hvapt	20.90	kJ/mol	205.50	NIST Webbook
hvapt	19.40 ± 0.10	kJ/mol	234.00	NIST Webbook
pvap	594.92	kPa	283.15	Measurements of Bubble Point Pressures for the Binary Mixture of Pentafluoroethane with Chloropentafluoroethane
pvap	148.60	kPa	243.15	Measurements of Bubble Point Pressures for the Binary Mixture of Pentafluoroethane with Chloropentafluoroethane
pvap	1664.90	kPa	323.15	Measurements of Bubble Point Pressures for the Binary Mixture of Pentafluoroethane with Chloropentafluoroethane
pvap	1317.90	kPa	313.15	Measurements of Bubble Point Pressures for the Binary Mixture of Pentafluoroethane with Chloropentafluoroethane
pvap	219.90	kPa	253.15	Measurements of Bubble Point Pressures for the Binary Mixture of Pentafluoroethane with Chloropentafluoroethane
pvap	314.60	kPa	263.15	Measurements of Bubble Point Pressures for the Binary Mixture of Pentafluoroethane with Chloropentafluoroethane
pvap	439.40	kPa	273.15	Measurements of Bubble Point Pressures for the Binary Mixture of Pentafluoroethane with Chloropentafluoroethane

pvap	1028.40	kPa	303.15	Measurements of Bubble Point Pressures for the Binary Mixture of Pentafluoroethane with Chloropentafluoroethane
pvap	789.30	kPa	293.15	Measurements of Bubble Point Pressures for the Binary Mixture of Pentafluoroethane with Chloropentafluoroethane
pvap	2077.50	kPa	333.15	Measurements of Bubble Point Pressures for the Binary Mixture of Pentafluoroethane with Chloropentafluoroethane
rhol	1260.00	kg/m3	303.00	KDB
sfust	10.79	J/mol×K	173.70	NIST Webbook
sfust	32.76	J/mol×K	80.24	NIST Webbook
srf	0.01	N/m	298.20	KDB
svapt	82.93	J/mol×K	234.04	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.38962e+01
Coeff. B	-1.96705e+03
Coeff. C	-2.34850e+01
Temperature range (K), min.	168.03
Temperature range (K), max.	353.10

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	6.94742e+01
Coeff. B	-4.08741e+03
Coeff. C	-8.85890e+00
Coeff. D	1.71756e-05
Temperature range (K), min.	174.00

Temperature range (K), max.	353.00

Sources

Measurements of Bubble Point Pressures for the Binary Mixture of Pentafluoroethane with Chloropentafluoroethane:	https://www.doi.org/10.1021/je400837p
KDB Vapor Pressure Data:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1535
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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C76153&Units=SI
KDB:	https://www.cheric.org/files/research/kdb/mol/mol1535.mol
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

Legend

af:	Acentric Factor
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
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
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