Dichlorodifluoromethane

Other names:

ARCTON 6
Algofrene Type 2
Arcton 12
CCl2F2
CF2Cl2
CFC-12
Chlorofluorocarbon 12
Chlorofluoromethane (CCl2F2)
Difluorodichloromethane
Dwuchlorodwufluorometan
Dymel 12
Electro-CF 12
Eskimon 12
F 12
FC 12
FCC 12
FKW 12
Fluorocarbon 12
Forane 12
Freon 12
Freon F-12
Frigen 12
Genetron 12
Halocarbon 12
Halon 122
Isceon 122
Isotron 12
Isotron 2
Kaiser chemicals 12
Ledon 12
Methane, dichlorodifluoro-
Propellant 12
Propellent 12
R 12
R 12, Refrigerant
R-12
REFRIGERANT-12
Rcra waste number U075
Refrigerant 12
Refrigerant R12

	UN 1028
	Ucon 12
	Ucon 12/halocarbon 12
Inchi:	InChI=1S/CCl2F2/c2-1(3,4)5
InchiKey:	PXBRQCKWGAHEHS-UHFFFAOYSA-N
Formula:	CCl2F2
SMILES:	FC(F)(Cl)Cl
Mol. weight [g/mol]:	120.91
CAS:	75-71-8

Physical Properties

Property code	Value	Unit	Source
af	0.2040		KDB
dm	0.50	debye	KDB
ea	0.40 ± 0.20	eV	NIST Webbook
gf	-442.50	kJ/mol	KDB
hf	-477.60 ± 5.60	kJ/mol	NIST Webbook
hf	-481.50	kJ/mol	KDB
hf	-469.00 ± 8.00	kJ/mol	NIST Webbook
hf	-477.00 ± 13.00	kJ/mol	NIST Webbook
hfus	5.49	kJ/mol	Joback Method
hvap	23.66	kJ/mol	Joback Method
ie	11.87 ± 0.02	eV	NIST Webbook
ie	11.70 ± 0.50	eV	NIST Webbook
ie	12.24 ± 0.01	eV	NIST Webbook
ie	12.00 ± 0.20	eV	NIST Webbook
ie	11.75	eV	NIST Webbook
ie	12.31 ± 0.05	eV	NIST Webbook
ie	12.26 ± 0.02	eV	NIST Webbook
ie	11.75 ± 0.04	eV	NIST Webbook
ie	12.30	eV	NIST Webbook
log10ws	-1.99		Aqueous Solubility Prediction Method
logp	2.014		Crippen Method
mcvol	52.970	ml/mol	McGowan Method
pc	4136.00	kPa	KDB
pc	4129.00 ± 15.00	kPa	NIST Webbook
pc	4116.15	kPa	NIST Webbook
pc	3911.15 ± 6.07	kPa	NIST Webbook
pc	4131.00 ± 5.00	kPa	NIST Webbook

pc	4119.00 ± 20.00	kPa	NIST Webbook
pt	0.01 ± 0.01	kPa	NIST Webbook
rhoc	579.06 ± 0.48	kg/m3	NIST Webbook
rhoc	669.86 ± 8.46	kg/m3	NIST Webbook
rhoc	568.30 ± 5.67	kg/m3	NIST Webbook
rhoc	568.30 ± 4.84	kg/m3	NIST Webbook
rinpol	305.00		NIST Webbook
rinpol	305.00		NIST Webbook
rinpol	313.00		NIST Webbook
rinpol	318.00		NIST Webbook
rinpol	313.00		NIST Webbook
rinpol	305.00		NIST Webbook
rinpol	320.00		NIST Webbook
rinpol	311.00		NIST Webbook
rinpol	314.00		NIST Webbook
rinpol	318.00		NIST Webbook
rinpol	314.00		NIST Webbook
tb	243.30	K	KDB
tc	385.15 ± 0.30	K	NIST Webbook
tc	385.15 ± 0.20	K	NIST Webbook
tc	385.15	K	NIST Webbook
tc	385.01 ± 0.05	K	NIST Webbook
tc	385.01 ± 0.03	K	NIST Webbook
tc	384.95	K	KDB
tc	302.30 ± 0.06	K	NIST Webbook
tf	115.37	K	NIST Webbook
tf	115.00	K	KDB
tf	115.20 ± 0.30	K	NIST Webbook
tt	390.35 ± 0.05	K	NIST Webbook
tt	116.10 ± 0.01	K	NIST Webbook
tt	115.15 ± 0.10	K	NIST Webbook
vc	0.217	m3/kmol	KDB
zc	0.2804140		KDB
zra	0.28		KDB

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	70.97	J/mol×K	292.45	Joback Method
cpg	85.57	J/mol×K	435.79	Joback Method
cpg	83.18	J/mol×K	407.12	Joback Method

cpg	80.54	J/mol×K	378.45	Joback Method
cpg	77.63	J/mol×K	349.78	Joback Method
cpg	74.45	J/mol×K	321.12	Joback Method
cpg	87.73	J/mol×K	464.45	Joback Method
cpl	126.80	J/mol×K	290.00	NIST Webbook
hvapt	19.97	kJ/mol	243.30	KDB
hvapt	20.40	kJ/mol	243.00	NIST Webbook
hvapt	21.50	kJ/mol	198.50	NIST Webbook
hvapt	22.90	kJ/mol	225.50	NIST Webbook
hvapt	20.50	kJ/mol	363.00	NIST Webbook
hvapt	20.40	kJ/mol	260.50	NIST Webbook
hvapt	21.60	kJ/mol	206.50	NIST Webbook
hvapt	21.40	kJ/mol	208.50	NIST Webbook
hvapt	20.00	kJ/mol	313.50	NIST Webbook
rhol	1750.00	kg/m3	158.00	KDB
srf	0.01	N/m	277.60	KDB

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.39235e+01
Coeff. B	-1.99245e+03
Coeff. C	-2.92770e+01
Temperature range (K), min.	175.40
Temperature range (K), max.	385.12

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	9.22643e+01
Coeff. B	-4.84972e+03
Coeff. C	-1.25836e+01
Coeff. D	2.42960e-05
Temperature range (K), min.	115.15
Temperature range (K), max.	384.95

Sources

Measurement of gas mixing volumes by Flux Response Technology:	https://www.doi.org/10.1016/j.fluid.2006.11.004
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
KDB:	https://www.cheric.org/files/research/kdb/mol/mol1506.mol
KDB Vapor Pressure Data:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1506
Determination of Dichlorodifluoromethane's Diffusion Coefficients in Hydrogen, Helium, Nitrogen, and Air by Reversed-Flow Inverse Gas Chromatography:	https://www.doi.org/10.1021/acs.jced.8b01229
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C75718&Units=SI
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Determination of Henry's Law Constants Using Internal Standards with Benchmark Values:	https://www.doi.org/10.1021/je3010535
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
KDB Pure (Korean Thermophysical Properties Databank):	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1506

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
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
pt:	Triple Point Pressure
pvap:	Vapor pressure
rhoc:	Critical density
rhol:	Liquid Density
rinpol:	Non-polar retention indices
srf:	Surface Tension
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