

Ethane, 1,1,2,2-tetrachloro-1,2-difluoro-

Other names:	1,1,2,2-TETRACHLORODIFLUOROETHANE 1,1,2,2-Tetrachloro-1,2-difluoroethane 1,2-Difluoro-1,1,2,2-tetrachloroethane 1,2-Difluorotetrachloroethane CFCI2CFCI2 Daiflon 112 Daiflon S2 Difluorotetrachloroethane Ethane, 1,2-difluoro-1,1,2,2-tetrachloro- F-112 FC 112 FREON 112 Freon R 112 Genetron 112 Halocarbon 112 R 112 Refrigerant 112 S-TETRACHLORODIFLUOROETHANE Tetrachloro-1,2-Difluoroethane Ucon 112 sym-Tetrachlorodifluoroethane
Inchi:	InChI=1S/C2Cl4F2/c3-1(4,7)2(5,6)8
InchiKey:	UGCSPKPEHQEOSR-UHFFFAOYSA-N
Formula:	C2Cl4F2
SMILES:	FC(Cl)(Cl)C(F)(Cl)Cl
Mol. weight [g/mol]:	203.83
CAS:	76-12-0

Physical Properties

Property code	Value	Unit	Source
gf	-465.70	kJ/mol	Joback Method
hf	-557.29	kJ/mol	Joback Method
hfus	9.06	kJ/mol	Joback Method
hvap	32.70	kJ/mol	NIST Webbook
hvap	34.80 ± 0.40	kJ/mol	NIST Webbook
ie	11.60	eV	NIST Webbook

ie	11.30	eV	NIST Webbook
log10ws	-3.18		Crippen Method
logp	3.188		Crippen Method
mcvol	91.540	ml/mol	McGowan Method
pc	3857.88	kPa	Joback Method
rinpol	702.10		NIST Webbook
rinpol	704.00		NIST Webbook
rinpol	694.00		NIST Webbook
rinpol	704.00		NIST Webbook
rinpol	702.10		NIST Webbook
rinpol	709.00		NIST Webbook
rinpol	691.00		NIST Webbook
rinpol	681.00		NIST Webbook
ripol	888.00		NIST Webbook
ripol	870.00		NIST Webbook
ripol	870.00		NIST Webbook
sl	283.43	J/molxK	NIST Webbook
sl	273.84	J/molxK	NIST Webbook
tb	364.70 ± 4.00	K	NIST Webbook
tb	365.95	K	KDB
tb	365.90	K	NIST Webbook
tb	366.20	K	NIST Webbook
tb	365.75 ± 0.40	K	NIST Webbook
tc	592.71	K	Joback Method
tf	238.00	K	Joback Method
tt	299.70 ± 0.02	K	NIST Webbook
tt	297.91 ± 0.01	K	NIST Webbook
tt	297.91	K	KDB
vc	0.357	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	152.57	J/molxK	489.84	Joback Method
cpg	143.76	J/molxK	421.25	Joback Method
cpg	138.37	J/molxK	386.96	Joback Method
cpg	156.09	J/molxK	524.13	Joback Method
cpg	159.09	J/molxK	558.42	Joback Method
cpg	161.61	J/molxK	592.71	Joback Method
cpg	148.47	J/molxK	455.54	Joback Method
cpl	173.60	J/molxK	298.00	NIST Webbook

cpl	178.59	J/mol×K	300.00	NIST Webbook
cpl	175.52	J/mol×K	298.15	NIST Webbook
hfust	3.67	kJ/mol	297.91	NIST Webbook
hfust	3.70	kJ/mol	299.70	NIST Webbook
hfust	3.70	kJ/mol	299.70	NIST Webbook
hfust	0.79	kJ/mol	130.00	NIST Webbook
hfust	3.70	kJ/mol	299.70	NIST Webbook
hsubt	36.40	kJ/mol	264.00	NIST Webbook
hsubt	38.20	kJ/mol	265.00	NIST Webbook
hvapt	35.17	kJ/mol	366.20	NIST Webbook
hvapt	34.60 ± 0.10	kJ/mol	308.00	NIST Webbook
hvapt	34.10 ± 0.10	kJ/mol	315.00	NIST Webbook
hvapt	33.60 ± 0.10	kJ/mol	323.00	NIST Webbook
hvapt	34.00	kJ/mol	337.00	NIST Webbook
hvapt	36.40	kJ/mol	264.00	NIST Webbook
hvapt	36.60	kJ/mol	333.00	NIST Webbook
hvapt	32.60 ± 0.10	kJ/mol	338.00	NIST Webbook
hvapt	33.10 ± 0.10	kJ/mol	330.00	NIST Webbook
sfust	12.31	J/mol×K	297.91	NIST Webbook
sfust	12.33	J/mol×K	299.70	NIST Webbook
sfust	6.08	J/mol×K	130.00	NIST Webbook
sfust	12.35	J/mol×K	299.70	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.40018e+01
Coeff. B	-2.92421e+03
Coeff. C	-5.43650e+01
Temperature range (K), min.	267.59
Temperature range (K), max.	390.86

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/T + C \cdot \ln(T) + D \cdot T^2$
Coeff. A	2.86377e+01
Coeff. B	-4.85447e+03
Coeff. C	-1.80130e+00

Coeff. D	-1.17110e-06
Temperature range (K), min.	283.00
Temperature range (K), max.	551.00

Sources

KDB:	https://www.thermochimica.org/files/research/kdb/mol/mol1541.mol
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C76120&Units=SI
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
KDB Vapor Pressure Data:	https://www.thermochimica.org/research/kdb/hcprop/showprop.php?cmpid=1541
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

cpg:	Ideal gas heat capacity
cpl:	Liquid phase heat capacity
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
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
rinpolar:	Non-polar retention indices
ripolar:	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

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