

Methane, chlorofluoro-

Other names:	CFC 31 CH2CIF CH2FCI Chlorofluoromethane FC 31 FREON 31 HCFC 31 Methylene chloride fluoride Monochloromonofluoromethane R 31 R 31 (refrigerant) REFRIGERANT-31
Inchi:	InChI=1S/CH2CIF/c2-1-3/h1H2
InchiKey:	XWCDSDSNJVCLO-UHFFFAOYSA-N
Formula:	CH2CIF
SMILES:	FCCI
Mol. weight [g/mol]:	68.48
CAS:	593-70-4

Physical Properties

Property code	Value	Unit	Source
af	0.1990		KDB
gf	-249.20	kJ/mol	Joback Method
hf	-275.82	kJ/mol	Joback Method
hfus	5.62	kJ/mol	Joback Method
hvap	21.39	kJ/mol	Joback Method
ie	11.74	eV	NIST Webbook
ie	11.71 ± 0.01	eV	NIST Webbook
log10ws	-0.74		Crippen Method
logp	1.152		Crippen Method
mcvol	38.960	ml/mol	McGowan Method
pc	5130.00	kPa	KDB
rinpol	374.00		NIST Webbook
rinpol	374.00		NIST Webbook
tb	264.00	K	NIST Webbook
tb	264.10	K	KDB
tc	424.90	K	KDB

tf	140.00	K	KDB
vc	0.159	m ³ /kmol	KDB
zc	0.2301560		KDB

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	47.11	J/mol×K	258.98	Joback Method
cpg	49.32	J/mol×K	285.27	Joback Method
cpg	51.46	J/mol×K	311.57	Joback Method
cpg	53.52	J/mol×K	337.86	Joback Method
cpg	55.51	J/mol×K	364.15	Joback Method
cpg	57.44	J/mol×K	390.45	Joback Method
cpg	59.29	J/mol×K	416.74	Joback Method
hvapt	23.30	kJ/mol	202.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.45553e+01
Coeff. B	-2.37042e+03
Coeff. C	-2.54550e+01
Temperature range (K), min.	191.59
Temperature range (K), max.	281.97

Sources

The Yaws Handbook of Vapor

Pressure:
Crippen Method:

Crippen Method:

Joback Method:

KDB:

McGowan Method:

<https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure>

<http://pubs.acs.org/doi/abs/10.1021/ci9903071>

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

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

<https://www.thermo.com/files/research/kdb/mol/mol1525.mol>

<http://link.springer.com/article/10.1007/BF02311772>

Legend

af:	Acentric Factor
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
mccvol:	McGowan's characteristic volume
pc:	Critical Pressure
pvap:	Vapor pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume
zc:	Critical Compressibility

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