

Ethene, 1-chloro-1-fluoro-

Other names:	Ethylene, 1-chloro-1-fluoro- 1-Chloro-1-fluoroethylene CH2=CFCI
Inchi:	InChI=1S/C2H2CIF/c1-2(3)4/h1H2
InchiKey:	FPBWSPZHCJXUBL-UHFFFAOYSA-N
Formula:	C2H2CIF
SMILES:	C=C(F)CI
Mol. weight [g/mol]:	80.49
CAS:	2317-91-1

Physical Properties

Property code	Value	Unit	Source
gf	-161.49	kJ/mol	Joback Method
hf	-180.82	kJ/mol	Joback Method
hfus	5.62	kJ/mol	Joback Method
hvap	23.02	kJ/mol	Joback Method
ie	10.70 ± 0.20	eV	NIST Webbook
ie	10.70 ± 0.20	eV	NIST Webbook
ie	9.97	eV	NIST Webbook
log10ws	-1.51		Crippen Method
logp	1.666		Crippen Method
mcvol	48.750	ml/mol	McGowan Method
pc	4789.21	kPa	Joback Method
rinpol	375.00		NIST Webbook
rinpol	375.00		NIST Webbook
tb	249.00 ± 1.50	K	NIST Webbook
tb	249.00	K	NIST Webbook
tc	445.44	K	Joback Method
tf	127.09	K	Joback Method
vc	0.197	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
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cpg	60.52	J/mol×K	278.42	Joback Method
cpg	63.81	J/mol×K	306.26	Joback Method
cpg	66.94	J/mol×K	334.09	Joback Method
cpg	69.91	J/mol×K	361.93	Joback Method
cpg	72.74	J/mol×K	389.76	Joback Method
cpg	75.42	J/mol×K	417.60	Joback Method
cpg	77.96	J/mol×K	445.44	Joback Method

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C2317911&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

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
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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