Benzene, 1-chloro-3-fluoro-

Other names:	1-Chloro-3-fluorobenzene
	1-Fluoro-3-chlorobenzene
	3-Chlorofluorobenzene
	3-chloro-1-fluorobenzene
	m-Chlorofluorobenzene
	m-Fluorochlorobenzene
Inchi:	InChI=1S/C6H4ClF/c7-5-2-1-3-6(8)4-5/h1-4H
InchiKey:	VZHJIJZEOCBKRA-UHFFFAOYSA-N
Formula:	C6H4ClF
SMILES:	Fc1cccc(Cl)c1
Mol. weight [g/mol]:	130.55
CAS:	625-98-9

Physical Properties

Property code	Value	Unit	Source
gf	-104.32	kJ/mol	Joback Method
hf	-153.96	kJ/mol	Joback Method
hfus	12.22	kJ/mol	Joback Method
hvap	35.46	kJ/mol	Joback Method
ie	9.25	eV	NIST Webbook
ie	9.22 ± 0.02	eV	NIST Webbook
ie	9.21 ± 0.01	eV	NIST Webbook
log10ws	-2.49		Crippen Method
logp	2.479		Crippen Method
mcvol	85.650	ml/mol	McGowan Method
pc	4109.14	kPa	Joback Method
rinpol	812.00		NIST Webbook
rinpol	811.10		NIST Webbook
rinpol	811.10		NIST Webbook
rinpol	835.40		NIST Webbook
rinpol	811.10		NIST Webbook
tb	400.80	K	NIST Webbook
tb	400.00 ± 1.00	K	NIST Webbook
tc	616.31	K	Joback Method
tf	226.83	K	Joback Method
vc	0.331	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	166.45	J/mol×K	545.88	Joback Method
cpg	172.92	J/mol×K	581.09	Joback Method
cpg	135.91	J/mol×K	405.04	Joback Method
cpg	144.28	J/mol×K	440.25	Joback Method
cpg	152.15	J/mol×K	475.46	Joback Method
cpg	159.53	J/mol×K	510.67	Joback Method
cpg	178.96	J/mol×K	616.31	Joback Method
hvapt	43.00	kJ/mol	298.15	Vaporization enthalpies of a series of the halogen-substituted fluorobenzenes
hvapt	37.40	kJ/mol	338.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.60331e+01
Coeff. B	-4.61365e+03
Coeff. C	3.43200e+00
Temperature range (K), min.	273.00
Temperature range (K), max.	426.88

Sources

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=C625989&Units=SI

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

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Vaporization enthalpies of a series of the halogen-substituted fluorobenzenes:	https://www.doi.org/10.1016/j.fluid.2014.12.023

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
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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume