Benzene, 1-chloro-4-fluoro-

Other names:	1,4-Fluorochlorobenzene
	1-Fluoro-4-chlorobenzene
	1-chloro-4-fluorobenzene
	4-Chlorofluorobenzene
	4-chloro-1-fluorobenzene
	p-Chlorofluorobenzene
	p-Fluorochlorobenzene
Inchi:	InChI=1S/C6H4ClF/c7-5-1-3-6(8)4-2-5/h1-4H
InchiKey:	RJCGZNCCVKIBHO-UHFFFAOYSA-N
Formula:	C6H4ClF
SMILES:	Fc1ccc(Cl)cc1
Mol. weight [g/mol]:	130.55
CAS:	352-33-0

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
hsub	71.86 ± 0.21	kJ/mol	NIST Webbook
hsub	71.90 ± 0.40	kJ/mol	NIST Webbook
hvap	35.46	kJ/mol	Joback Method
ie	9.05	eV	NIST Webbook
ie	9.26	eV	NIST Webbook
ie	9.01 ± 0.01	eV	NIST Webbook
ie	9.08 ± 0.02	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	840.50		NIST Webbook
rinpol	827.00		NIST Webbook
rinpol	840.50		NIST Webbook
rinpol	827.00		NIST Webbook
tb	402.50 ± 0.50	K	NIST Webbook
tb	402.70	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	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	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	178.96	J/mol×K	616.31	Joback Method
hfust	13.90	kJ/mol	245.00	NIST Webbook
hfust	16.10	kJ/mol	326.70	NIST Webbook
hsubt	61.10 ± 0.60	kJ/mol	313.00	NIST Webbook
hvapt	42.80	kJ/mol	298.15	Vaporization enthalpies of a series of the halogen-substituted fluorobenzenes
hvapt	56.50	kJ/mol	416.50	NIST Webbook

Sources

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
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=C352330&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
hfust:	Enthalpy of fusion at a given temperature
hsub:	Enthalpy of sublimation at standard conditions
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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

Latest version available from:

https://www.chemeo.com/cid/61-138-1/Benzene-1-chloro-4-fluoro.pdf

Generated by Cheméo on 2024-10-12 02:53:04.439240358 +0000 UTC m=+3282447.076209606.

Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.