Benzene, 1-fluoro-2-methyl-

Other names:	1-FLUORO-2-METHYLBENZENE
	1-Methyl-2-fluorobenzene
	2-FLUOROTOLUENE
	Toluene, 2-fluoro
	Toluene, o-fluoro-
	UN 2388
	o-Fluorotoluene
	ortho-Fluorotoluene
Inchi:	InChI=1S/C7H7F/c1-6-4-2-3-5-7(6)8/h2-5H,1H3
InchiKey:	MMZYCBHLNZVROM-UHFFFAOYSA-N
Formula:	C7H7F
SMILES:	Cc1ccccc1F
Mol. weight [g/mol]:	110.13
CAS:	95-52-3

Physical Properties

Property code	Value	Unit	Source
affp	773.30	kJ/mol	NIST Webbook
basg	743.80	kJ/mol	NIST Webbook
chl	-3779.00	kJ/mol	NIST Webbook
gf	-83.97	kJ/mol	Joback Method
hf	-158.86	kJ/mol	Joback Method
hfus	10.62	kJ/mol	Joback Method
hvap	33.30	kJ/mol	Joback Method
ie	8.92 ± 0.01	eV	NIST Webbook
ie	8.91 ± 0.01	eV	NIST Webbook
ie	8.91 ± 0.01	eV	NIST Webbook
log10ws	-2.28		Crippen Method
logp	2.134		Crippen Method
mcvol	87.500	ml/mol	McGowan Method
pc	3815.10	kPa	Joback Method
rinpol	777.40		NIST Webbook
rinpol	783.00		NIST Webbook
rinpol	763.70		NIST Webbook
rinpol	767.00		NIST Webbook
rinpol	783.00		NIST Webbook
rinpol	777.40		NIST Webbook

rinpol	757.00		NIST Webbook
rinpol	777.00		NIST Webbook
rinpol	767.00		NIST Webbook
rinpol	785.00		NIST Webbook
rinpol	757.00		NIST Webbook
rinpol	777.00		NIST Webbook
rinpol	767.00		NIST Webbook
tb	387.20	K	NIST Webbook
tb	387.00	K	NIST Webbook
tc	591.59	K	Joback Method
tf	208.18	K	Joback Method
vc	0.338	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	201.85	J/mol×K	591.59	Joback Method
cpg	158.20	J/mol×K	424.01	Joback Method
cpg	167.93	J/mol×K	457.52	Joback Method
cpg	177.14	J/mol×K	491.04	Joback Method
cpg	185.85	J/mol×K	524.56	Joback Method
cpg	194.09	J/mol×K	558.07	Joback Method
cpg	147.93	J/mol×K	390.49	Joback Method
hfust	9.80	kJ/mol	204.00	NIST Webbook
hfust	9.80	kJ/mol	210.65	NIST Webbook
hfust	9.80	kJ/mol	210.70	NIST Webbook
hfust	9.80	kJ/mol	210.70	NIST Webbook
hvapt	42.00	kJ/mol	318.00	NIST Webbook
hvapt	31.50	kJ/mol	491.50	NIST Webbook
hvapt	38.70	kJ/mol	341.50	NIST Webbook
hvapt	32.30	kJ/mol	491.50	NIST Webbook
hvapt	38.00	kJ/mol	328.00	NIST Webbook
hvapt	40.50	kJ/mol	317.50	NIST Webbook
sfust	46.00	J/mol×K	210.65	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source

tbrp	303.20	K	3.50	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.45689e+01
Coeff. B	-3.36273e+03
Coeff. C	-4.90560e+01
Temperature range (K), min.	284.52
Temperature range (K), max.	412.30

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	8.37638e+01
Coeff. B	-7.26236e+03
Coeff. C	-1.03591e+01
Coeff. D	8.94046e-06
Temperature range (K), min.	249.15
Temperature range (K), max.	417.15

Sources

KDB: https://www.cheric.org/files/research/kdb/mol/mol1705.mol

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C95523&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.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1705

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

affp:	Proton affinity
basg:	Gas basicity
chl:	Standard liquid enthalpy of combustion
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
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
sfust:	Entropy of fusion at a given temperature
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume