Benzene, 1-fluoro-4-methyl-

Other names:	1-FLUORO-4-METHYLBENZENE
	1-Methyl-4-fluorobenzene
	4-FLUOROTOLUENE
	NSC 8861
	Toluene, 4-fluoro
	Toluene, p-fluoro-
	p-Fluoromethylbenzene
	p-Fluorotoluene
	para-Fluorotoluene
Inchi:	InChI=1S/C7H7F/c1-6-2-4-7(8)5-3-6/h2-5H,1H3
InchiKey:	WRWPPGUCZBJXKX-UHFFFAOYSA-N
Formula:	C7H7F
SMILES:	Cc1ccc(F)cc1
Mol. weight [g/mol]:	110.13
CAS:	352-32-9

Physical Properties

Property code	Value	Unit	Source
affp	763.80	kJ/mol	NIST Webbook
basg	736.10	kJ/mol	NIST Webbook
chl	-3777.90	kJ/mol	NIST Webbook
chl	-3747.20 ± 0.71	kJ/mol	NIST Webbook
gf	-83.97	kJ/mol	Joback Method
hf	-147.50 ± 0.08	kJ/mol	NIST Webbook
hfl	-186.90 ± 0.08	kJ/mol	NIST Webbook
hfus	10.62	kJ/mol	Joback Method
hvap	39.50	kJ/mol	NIST Webbook
hvap	39.40 ± 0.08	kJ/mol	NIST Webbook
hvap	39.47	kJ/mol	NIST Webbook
ie	8.79 ± 0.01	eV	NIST Webbook
ie	8.79 ± 0.01	eV	NIST Webbook
ie	8.79 ± 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	787.00		NIST Webbook

rinpol	770.40		NIST Webbook
rinpol	756.00		NIST Webbook
rinpol	775.00		NIST Webbook
rinpol	777.70		NIST Webbook
rinpol	777.70		NIST Webbook
rinpol	775.00		NIST Webbook
rinpol	775.00		NIST Webbook
sl	237.11	J/mol×K	NIST Webbook
tb	389.00	K	NIST Webbook
tb	389.80	K	NIST Webbook
tb	389.80	K	NIST Webbook
tc	589.50	K	NIST Webbook
tf	215.60 ± 0.20	K	NIST Webbook
tt	216.48 ± 0.01	K	NIST Webbook
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	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
cpg	158.20	J/mol×K	424.01	Joback Method
cpg	167.93	J/mol×K	457.52	Joback Method
cpl	171.17	J/mol×K	298.15	NIST Webbook
cpl	172.30	J/mol×K	298.15	NIST Webbook
cpl	173.70	J/mol×K	298.15	NIST Webbook
hfust	7.65	kJ/mol	213.00	NIST Webbook
hfust	9.35	kJ/mol	216.49	NIST Webbook
hfust	9.35	kJ/mol	216.50	NIST Webbook
hfust	9.35	kJ/mol	216.50	NIST Webbook
hfust	8.80	kJ/mol	215.55	NIST Webbook
hvapt	37.00	kJ/mol	384.50	NIST Webbook
hvapt	34.08	kJ/mol	389.80	NIST Webbook
sfust	43.19	J/mol×K	216.49	NIST Webbook
sfust	41.00	J/mol×K	215.55	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.44160e+01
Coeff. B	-3.32702e+03
Coeff. C	-5.02270e+01
Temperature range (K), min.	285.71
Temperature range (K), max.	415.65

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	7.64576e+01
Coeff. B	-7.14432e+03
Coeff. C	-9.12454e+00
Coeff. D	6.06129e-06
Temperature range (K), min.	340.15
Temperature range (K), max.	590.48

Sources

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

KDB: https://www.cheric.org/files/research/kdb/mol/mol1707.mol

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C352329&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=1707

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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

Legend

affp: Proton affinity

basg:	Gas basicity
chl:	Standard liquid enthalpy of combustion
cpg:	Ideal gas heat capacity
cpl:	Liquid phase heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfl:	Liquid phase 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
sl:	Liquid phase molar entropy at standard conditions
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
tt:	Triple Point Temperature
vc:	Critical Volume