Benzene, fluoro-

Other names:	Fluorobenzene
	Fluorobenzenes
	Monofluorobenzene
	PHENYL FLUORIDE
	UN 2387
Inchi:	InChI=1S/C6H5F/c7-6-4-2-1-3-5-6/h1-5H
InchiKey:	PYLWMHQQBFSUBP-UHFFFAOYSA-N
Formula:	C6H5F
SMILES:	Fc1ccccc1
Mol. weight [g/mol]:	96.10
CAS:	462-06-6

Physical Properties

Property code	Value	Unit	Source
af	0.2440		KDB
affp	755.90	kJ/mol	NIST Webbook
basg	726.60	kJ/mol	NIST Webbook
chl	-3103.90 ± 1.20	kJ/mol	NIST Webbook
chl	-3126.00	kJ/mol	NIST Webbook
dm	1.40	debye	KDB
gf	-69.08	kJ/mol	KDB
hf	-116.60	kJ/mol	KDB
hfl	-150.80 ± 1.40	kJ/mol	NIST Webbook
hfus	8.42	kJ/mol	Joback Method
hvap	34.60	kJ/mol	NIST Webbook
hvap	34.53	kJ/mol	NIST Webbook
hvap	34.68	kJ/mol	NIST Webbook
hvap	34.50	kJ/mol	NIST Webbook
ie	9.19	eV	NIST Webbook
ie	9.35 ± 0.03	eV	NIST Webbook
ie	9.20 ± 0.01	eV	NIST Webbook
ie	9.20	eV	NIST Webbook
ie	9.20 ± 0.01	eV	NIST Webbook
ie	9.21 ± 0.04	eV	NIST Webbook
ie	9.22	eV	NIST Webbook
ie	9.20	eV	NIST Webbook
ie	9.20	eV	NIST Webbook

ie	9.11	eV	NIST Webbook
ie	9.75	eV	NIST Webbook
ie	9.17	eV	NIST Webbook
ie	9.20	eV	NIST Webbook
ie	9.20	eV	NIST Webbook
ie	9.20 ± 0.01	eV	NIST Webbook
ie	9.22	eV	NIST Webbook
ie	9.18	eV	NIST Webbook
ie	9.37	eV	NIST Webbook
log10ws	-1.80		Aqueous Solubility Prediction Method
log10ws	-1.80		Estimated Solubility Method
logp	1.826		Crippen Method
mcvol	73.410	ml/mol	McGowan Method
nfpaf	%!d(float64=3)		KDB
nfpah	%!d(float64=2)		KDB
nfpas	%!d(float64=3)		KDB
pc	4550.50 ± 5.06	kPa	NIST Webbook
pc	4521.23 ± 39.99	kPa	NIST Webbook
pc	4551.00	kPa	KDB
rinpol	666.00		NIST Webbook
rinpol	643.00		NIST Webbook
rinpol	664.90		NIST Webbook
rinpol	672.60		NIST Webbook
rinpol	684.00		NIST Webbook
rinpol	663.20		NIST Webbook
rinpol	681.00		NIST Webbook
rinpol	674.00		NIST Webbook
rinpol	668.00		NIST Webbook
rinpol	663.00		NIST Webbook
rinpol	664.00		NIST Webbook
rinpol	664.00		NIST Webbook
rinpol	673.90		NIST Webbook
rinpol	659.40		NIST Webbook
rinpol	674.00		NIST Webbook
rinpol	654.40		NIST Webbook
rinpol	674.00		NIST Webbook
rinpol	664.10		NIST Webbook
rinpol	681.00		NIST Webbook
rinpol	664.60		NIST Webbook
rinpol	651.30		NIST Webbook
rinpol	671.00		NIST Webbook
rinpol	680.00		NIST Webbook
rinpol	680.00		NIST Webbook

rinpol	671.50		NIST Webbook
ripol	992.00		NIST Webbook
ripol	996.00		NIST Webbook
sl	195.00	J/mol×K	NIST Webbook
sl	205.94	J/mol×K	NIST Webbook
tb	357.88	K	KDB
tc	560.10 ± 0.20	K	NIST Webbook
tc	557.30	K	The Critical Temperatures of a Number of (i) (Chloroalkane (C3 C4) + Hydrocarbon (C6 C7)) Binary Mixtures and (ii) (Aromatic Halocarbon (Chlorobenzene, Fluorobenzene, 1,2-Dichlorobenzene, or 1,3-Dichlorobenzene) + Alkane (C8)) Binary Mixtures
tc	560.10	K	NIST Webbook
tc	560.07 ± 0.07	K	NIST Webbook
tc	559.70 ± 0.60	K	NIST Webbook
tc	560.09	K	KDB
tf	231.25 ± 0.40	K	NIST Webbook
tf	230.94	K	KDB
tf	231.30 ± 1.00	K	NIST Webbook
tf	230.96 ± 0.06	K	NIST Webbook
tf	231.75	K	Aqueous Solubility Prediction Method
tf	231.25 ± 0.50	K	NIST Webbook
tt	230.92 ± 0.08	K	NIST Webbook
tt	231.10 ± 0.20	K	NIST Webbook
tt	230.94 ± 0.05	K	NIST Webbook
vc	0.462 ± 0.004	m3/kmol	NIST Webbook
vc	0.269	m3/kmol	KDB
vc	0.269 ± 0.008	m3/kmol	NIST Webbook
zc	0.2628840		KDB
zra	0.27		KDB

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	160.26	J/mol×K	563.38	Joback Method
cpg	146.03	J/mol×K	496.46	Joback Method
cpg	138.21	J/mol×K	463.01	Joback Method

cpg	129.89	J/mol×K	429.55	Joback Method
cpg	121.05	J/mol×K	396.09	Joback Method
cpg	111.67	J/mol×K	362.63	Joback Method
cpg	153.38	J/mol×K	529.92	Joback Method
cpl	146.57	J/mol×K	298.10	NIST Webbook
cpl	146.36	J/mol×K	298.15	NIST Webbook
cpl	146.29	J/mol×K	298.15	NIST Webbook
hfust	11.30	kJ/mol	230.94	NIST Webbook
hfust	11.31	kJ/mol	230.90	NIST Webbook
hfust	11.31	kJ/mol	230.90	NIST Webbook
hfust	10.40	kJ/mol	231.10	NIST Webbook
hvapt	31.19	kJ/mol	357.90	NIST Webbook
hvapt	32.40 ± 0.10	kJ/mol	337.00	NIST Webbook
hvapt	29.70 ± 0.10	kJ/mol	382.00	NIST Webbook
hvapt	33.50 ± 0.10	kJ/mol	318.00	NIST Webbook
hvapt	33.39	kJ/mol	358.10	KDB
hvapt	31.00	kJ/mol	457.50	NIST Webbook
hvapt	31.80	kJ/mol	396.00	NIST Webbook
hvapt	31.90	kJ/mol	444.00	NIST Webbook
hvapt	30.90	kJ/mol	529.00	NIST Webbook
hvapt	31.20 ± 0.10	kJ/mol	358.00	NIST Webbook
hvapt	33.60	kJ/mol	353.00	NIST Webbook
pvap	2.98	kPa	274.20	Vaporization enthalpies of a series of the fluoro- and chloro-substituted methylbenzenes
pvap	3.64	kPa	278.20	Vaporization enthalpies of a series of the fluoro- and chloro-substituted methylbenzenes
pvap	4.84	kPa	283.20	Vaporization enthalpies of a series of the fluoro- and chloro-substituted methylbenzenes
pvap	6.26	kPa	288.20	Vaporization enthalpies of a series of the fluoro- and chloro-substituted methylbenzenes
pvap	8.02	kPa	293.20	Vaporization enthalpies of a series of the fluoro- and chloro-substituted methylbenzenes

pvap	12.77	kPa	303.20	Vaporization enthalpies of a series of the fluoro- and chloro-substituted methylbenzenes
pvap	10.29	kPa	298.20	Vaporization enthalpies of a series of the fluoro- and chloro-substituted methylbenzenes
rfi	1.46300		303.15	Refractive properties, speed of sound and FT-IR study of binary mixtures of N-formylmorpholine with some halobenzenes at 303.15, 308.15 and 313.15 K
rfi	1.45940		308.15	Refractive properties, speed of sound and FT-IR study of binary mixtures of N-formylmorpholine with some halobenzenes at 303.15, 308.15 and 313.15 K
rfi	1.45630		313.15	Refractive properties, speed of sound and FT-IR study of binary mixtures of N-formylmorpholine with some halobenzenes at 303.15, 308.15 and 313.15 K
rfi	1.46290		298.15	Thermophysical properties of the binary mixtures of 2-methyl-tetrahydrofuran with benzene and halobenzenes
rhol	1024.96	kg/m3	293.15	The density, refractive index, and thermodynamic behaviour of binary mixtures of 1,3-Diethenyl-1,1,3,3-tetramethyldisiloxane with aromatic hydrocarbons

rhol	1022.27	kg/m3	293.20	Isobaric vapour liquid equilibria for binary mixtures of n-heptane with bromobenzene, chlorobenzene and fluorobenzene at atmospheric pressure
rhol	1036.89	kg/m3	283.15	The density, refractive index, and thermodynamic behaviour of binary mixtures of 1,3-Diethenyl-1,1,3,3-tetramethyldisiloxane with aromatic hydrocarbons
rhol	1030.93	kg/m3	288.15	The density, refractive index, and thermodynamic behaviour of binary mixtures of 1,3-Diethenyl-1,1,3,3-tetramethyldisiloxane with aromatic hydrocarbons
rhol	1024.00	kg/m3	293.00	KDB
rhol	1019.07	kg/m3	298.15	The density, refractive index, and thermodynamic behaviour of binary mixtures of 1,3-Diethenyl-1,1,3,3-tetramethyldisiloxane with aromatic hydrocarbons
rhol	985.00	kg/m3	330.10	Liquid-Liquid Equilibria in Binary Mixtures Containing Fluorinated Benzenes and Ionic Liquid 1-Ethyl-3-methylimidazolium Bis(trifluoromethylsulfonyl)imide
rhol	1022.27	kg/m3	293.20	Isobaric Vapor-Liquid Equilibria for Binary Mixtures of 1,2-Dibromoethane with Benzene, Toluene, Fluorobenzene, and Bromobenzene at Atmospheric Pressure

rhol	1022.00	kg/m3	296.20	Liquid-Liquid Equilibria in Binary Mixtures Containing Fluorinated Benzenes and Ionic Liquid 1-Ethyl-3-methylimidazolium Bis(trifluoromethylsulfonyl)imide
rhol	1013.03	kg/m3	303.15	The density, refractive index, and thermodynamic behaviour of binary mixtures of 1,3-Diethenyl-1,1,3,3-tetramethyldisiloxane with aromatic hydrocarbons
sfust	48.95	J/mol×K	230.94	NIST Webbook
sfust	44.99	J/mol×K	231.10	NIST Webbook
srf	0.03	N/m	293.20	KDB

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.43937e+01
Coeff. B	-3.10933e+03
Coeff. C	-3.99230e+01
Temperature range (K), min.	230.94
Temperature range (K), max.	382.28

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	6.12733e+01
Coeff. B	-5.96836e+03
Coeff. C	-6.90360e+00
Coeff. D	4.71669e-06
Temperature range (K), min.	230.94
Temperature range (K), max.	560.09

Sources

Solubility of Hydrofluorocarbons in Halobenzene Solvents:	https://www.doi.org/10.1021/je500525q
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Refractive properties, speed of sound and FT-IR study of binary mixtures of N-formylmorpholine with some halobenzenes at 303.15, 308.15 and 313.15 K:	https://www.doi.org/10.1016/j.fluid.2014.12.012
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
Thermophysical properties of the binary mixtures of 2-methyl-tetrahydrofuran with benzene and halobenzenes:	https://www.doi.org/10.1016/j.tca.2005.08.034
The Critical Temperatures of a Number of (i) (Chloroalkane (C3 C4) + Hydrocarbon (C6 C7)) Binary Mixtures and (ii) (Aromatic Halocarbon (Chlorobenzene, Fluorobenzene, 1,3-Dichlorobenzene) + Alkane (C8)) Binary Mixtures:	https://www.doi.org/10.1021/acs.jced.7b00191
Isobaric Vapor-Liquid Equilibria for Binary Mixtures of 1,2-Dibromoethane with Benzene, Toluene, Fluorobenzene, and Bromobenzene at Atmospheric Pressure:	https://www.doi.org/10.1021/je050231r
Abraham model correlations for describing the thermodynamic properties of solute transfer into pentyl acetate based on headspace chromatographic and solubility measurements:	https://www.doi.org/10.1016/j.jct.2018.05.003
Phase behavior of ionic liquids 1-alkyl-3-methylimidazolium bis(trifluoromethylsulfonyl)imides with fluorobenzenes:	https://www.doi.org/10.1016/j.jct.2015.04.012
KDB (Korean Thermophysical Properties Databank):	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1685
KDB Vapor Pressure Data:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1685
Liquid-Liquid Equilibria in Binary Mixtures Containing Fluorinated Benzenes and Ionic Liquid 1-Ethyl-3-methylimidazolium Bis(trifluoromethylsulfonyl)imide:	https://www.doi.org/10.1021/je8006474
Vaporization enthalpies of a series of the fluoro- and chloro-substituted methylbenzenes:	https://www.doi.org/10.1016/j.fluid.2014.07.029
Measurements and Calculation of Vapor-Liquid Equilibria for the Binary Mixtures of Fluorobenzene and Alkanes at a Pressure of 101.4 kPa:	https://www.doi.org/10.1021/je700207q
Quantitative Determination of Binodal and Phase Equilibrium Diagrams for the Ternary System (Fluorobenzene + Water + 2-Propanol) at Three Temperatures:	https://www.doi.org/10.1021/je700212q
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C462066&Units=SI
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
The density, refractive index, and thermodynamic behaviour of binary mixtures of 1,3-Diethenyl-1,1,3,3-tetramethyldisiloxane with aromatic hydrocarbons:	https://www.doi.org/10.1016/j.jct.2013.12.025
Estimated Solubility Method:	http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt
Isobaric vapour liquid equilibria for binary mixtures of n-heptane with bromobenzene, chlorobenzene and fluorobenzene at atmospheric pressure:	https://www.doi.org/10.1016/j.fluid.2005.11.020
KDB:	https://www.cheric.org/files/research/kdb/mol/mol1685.mol
Thermodynamics of solvation in propylene glycol and methyl cellosolve:	https://www.doi.org/10.1016/j.jct.2014.06.006

Legend

af:	Acentric Factor
affp:	Proton affinity
basg:	Gas basicity
chl:	Standard liquid enthalpy of combustion
cpg:	Ideal gas heat capacity
cpl:	Liquid phase heat capacity
dm:	Dipole Moment
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
nfpaf:	NFPA Fire Rating
nfpah:	NFPA Health Rating
nfpas:	NFPA Safety Rating
pc:	Critical Pressure
pvap:	Vapor pressure
rfi:	Refractive Index
rhol:	Liquid Density
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
sfust:	Entropy of fusion at a given temperature
sl:	Liquid phase molar entropy at standard conditions
srf:	Surface Tension
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
tt:	Triple Point Temperature
vc:	Critical Volume
zc:	Critical Compressibility
zra:	Rackett Parameter