Benzene, hexafluoro-

Other names:	1,2,3,4,5,6-HEXAFLUOROBENZENE
	CP 28
	Hexafluorobenzene
	PERFLUOROBENZENE
Inchi:	InChI=1S/C6F6/c7-1-2(8)4(10)6(12)5(11)3(1)9
InchiKey:	ZQBFAOFFOQMSGJ-UHFFFAOYSA-N
Formula:	C6F6
SMILES:	Fc1c(F)c(F)c(F)c(F)c1F
Mol. weight [g/mol]:	186.05
CAS:	392-56-3

Physical Properties

Property code	Value	Unit	Source
af	0.3960		KDB
affp	648.00	kJ/mol	NIST Webbook
basg	624.40	kJ/mol	NIST Webbook
chl	-2041.00 ± 8.40	kJ/mol	NIST Webbook
chl	-2443.60 ± 1.20	kJ/mol	NIST Webbook
cpl	221.42	J/mol×K	Reassembling and testing of a high-precision heat capacity drop calorimeter. Heat capacity of some polyphenyls at T = 298.15 K
ea	0.86 ± 0.03	eV	NIST Webbook
ea	0.80 ± 0.10	eV	NIST Webbook
ea	0.48	eV	NIST Webbook
ea	0.83 ± 0.20	eV	NIST Webbook
ea	0.53 ± 0.05	eV	NIST Webbook
ea	1.20 ± 0.07	eV	NIST Webbook
ea	1.80 ± 0.30	eV	NIST Webbook
ea	0.70 ± 0.10	eV	NIST Webbook
ea	0.52 ± 0.11	eV	NIST Webbook
gf	-880.00	kJ/mol	KDB
hf	-956.00 ± 1.20	kJ/mol	NIST Webbook
hf	-957.30	kJ/mol	KDB
hfl	-991.70 ± 1.20	kJ/mol	NIST Webbook
hfus	21.87	kJ/mol	Joback Method
hvap	29.63	kJ/mol	Joback Method

ie	9.90 ± 0.04	eV	NIST Webbook
ie	10.09	eV	NIST Webbook
ie	10.09	eV	NIST Webbook
ie	9.90	eV	NIST Webbook
ie	9.88 ± 0.05	eV	NIST Webbook
ie	10.20 ± 0.10	eV	NIST Webbook
ie	9.93	eV	NIST Webbook
ie	9.90 ± 0.01	eV	NIST Webbook
ie	10.20	eV	NIST Webbook
ie	10.14	eV	NIST Webbook
ie	9.91	eV	NIST Webbook
ie	9.90 ± 0.05	eV	NIST Webbook
ie	9.91	eV	NIST Webbook
ie	9.80	eV	NIST Webbook
ie	9.97	eV	NIST Webbook
log10ws	-3.46		Crippen Method
logp	2.521		Crippen Method
mcvol	82.260	ml/mol	McGowan Method
pc	3273.00	kPa	KDB
rhoc	550.35 ± 0.54	kg/m3	NIST Webbook
rhoc	493.04 ± 4.91	kg/m3	NIST Webbook
rinpol	548.70		NIST Webbook
rinpol	576.00		NIST Webbook
rinpol	571.00		NIST Webbook
rinpol	569.00		NIST Webbook
rinpol	600.00		NIST Webbook
rinpol	609.00		NIST Webbook
rinpol	592.00		NIST Webbook
rinpol	600.00		NIST Webbook
rinpol	546.80		NIST Webbook
sl	279.91	J/mol×K	NIST Webbook
sl	280.79	J/mol×K	NIST Webbook
tb	353.41	K	KDB
tc	516.73	K	KDB
tf	278.50	K	KDB
tt	278.30 ± 0.02	K	NIST Webbook
tt	278.30	K	KDB
tt	278.25 ± 0.02	K	NIST Webbook
tt	278.14 ± 0.15	K	NIST Webbook
vc	0.335 ± 0.002	m3/kmol	NIST Webbook
vc	0.335	m3/kmol	KDB
zc	0.2552060		KDB

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	159.94	J/mol×K	383.88	Joback Method
cpg	183.41	J/mol×K	515.92	Joback Method
cpg	179.00	J/mol×K	489.51	Joback Method
cpg	187.66	J/mol×K	542.33	Joback Method
cpg	169.76	J/mol×K	436.70	Joback Method
cpg	174.45	J/mol×K	463.10	Joback Method
cpg	164.92	J/mol×K	410.29	Joback Method
cpl	225.03	J/mol×K	298.15	NIST Webbook
cpl	221.60	J/mol×K	298.15	NIST Webbook
cpl	221.30	J/mol×K	298.76	NIST Webbook
cpl	221.58	J/mol×K	298.15	NIST Webbook
cpl	221.58	J/mol×K	298.15	NIST Webbook
cpl	222.00	J/mol×K	300.00	NIST Webbook
hfust	11.59	kJ/mol	278.30	NIST Webbook
hfust	11.59	kJ/mol	278.25	NIST Webbook
hfust	11.59	kJ/mol	278.30	NIST Webbook
hfust	11.59	kJ/mol	278.30	NIST Webbook
hsubt	49.80	kJ/mol	253.00	NIST Webbook
hsubt	49.20	kJ/mol	246.50	NIST Webbook
hsubt	46.00	kJ/mol	316.00	NIST Webbook
hvapt	31.80	kJ/mol	459.50	NIST Webbook
hvapt	35.10	kJ/mol	324.50	NIST Webbook
hvapt	35.50	kJ/mol	325.50	NIST Webbook
hvapt	36.50	kJ/mol	331.00	NIST Webbook
hvapt	31.66	kJ/mol	353.30	NIST Webbook
hvapt	32.20	kJ/mol	439.50	NIST Webbook
hvapt	36.20	kJ/mol	299.50	NIST Webbook
hvapt	35.70	kJ/mol	308.00	NIST Webbook
hvapt	31.80	kJ/mol	487.50	NIST Webbook
hvapt	34.40	kJ/mol	347.00	NIST Webbook
hvapt	33.20	kJ/mol	368.50	NIST Webbook
hvapt	36.50	kJ/mol	316.00	NIST Webbook
hvapt	32.20	kJ/mol	423.00	NIST Webbook
hvapt	31.68	kJ/mol	353.40	KDB
kvisc	0.0000005	m2/s	308.15	Viscosities of Liquid Fluorocompounds
kvisc	0.0000004	m2/s	313.15	Viscosities of Liquid Fluorocompounds

kvisc	0.0000004	m2/s	318.15	Viscosities of Liquid Fluorocompounds
kvisc	0.0000005	m2/s	303.15	Viscosities of Liquid Fluorocompounds
kvisc	0.0000006	m2/s	298.15	Viscosities of Liquid Fluorocompounds
pvap	9.00	kPa	293.51	Densities and Vapor Pressures of Highly Fluorinated Compounds
pvap	11.16	kPa	297.98	Densities and Vapor Pressures of Highly Fluorinated Compounds
pvap	14.20	kPa	302.96	Densities and Vapor Pressures of Highly Fluorinated Compounds
pvap	6.90	kPa	288.23	Densities and Vapor Pressures of Highly Fluorinated Compounds
pvap	22.25	kPa	312.96	Densities and Vapor Pressures of Highly Fluorinated Compounds
pvap	27.56	kPa	317.96	Densities and Vapor Pressures of Highly Fluorinated Compounds
pvap	33.85	kPa	322.96	Densities and Vapor Pressures of Highly Fluorinated Compounds
pvap	41.16	kPa	327.95	Densities and Vapor Pressures of Highly Fluorinated Compounds
pvap	17.93	kPa	307.96	Densities and Vapor Pressures of Highly Fluorinated Compounds
pvap	49.95	kPa	333.01	Densities and Vapor Pressures of Highly Fluorinated Compounds

rhol	1548.50	kg/m3	323.83	Properties of Perfluorobenzene near the Critical Point
rhol	1499.40	kg/m3	343.88	Properties of Perfluorobenzene near the Critical Point
rhol	1450.50	kg/m3	363.85	Properties of Perfluorobenzene near the Critical Point
rhol	1397.90	kg/m3	383.91	Properties of Perfluorobenzene near the Critical Point
rhol	1342.10	kg/m3	403.92	Properties of Perfluorobenzene near the Critical Point
rhol	1281.20	kg/m3	423.93	Properties of Perfluorobenzene near the Critical Point
rhol	1605.40	kg/m3	298.79	Properties of Perfluorobenzene near the Critical Point
rhol	1135.30	kg/m3	463.89	Properties of Perfluorobenzene near the Critical Point
rhol	1037.10	kg/m3	483.90	Properties of Perfluorobenzene near the Critical Point
rhol	974.00	kg/m3	493.93	Properties of Perfluorobenzene near the Critical Point
rhol	892.30	kg/m3	503.88	Properties of Perfluorobenzene near the Critical Point
rhol	835.80	kg/m3	508.90	Properties of Perfluorobenzene near the Critical Point
rhol	744.60	kg/m3	513.91	Properties of Perfluorobenzene near the Critical Point
rhol	746.30	kg/m3	513.92	Properties of Perfluorobenzene near the Critical Point
rhol	670.30	kg/m3	515.98	Properties of Perfluorobenzene near the Critical Point

rhol	644.80	kg/m3	516.28	Properties of Perfluorobenzene near the Critical Point
rhol	1213.90	kg/m3	443.90	Properties of Perfluorobenzene near the Critical Point
rhol	610.10	kg/m3	516.57	Properties of Perfluorobenzene near the Critical Point
sfust	41.63	J/mol×K	278.30	NIST Webbook
sfust	41.65	J/mol×K	278.25	NIST Webbook
srf	0.02	N/m	308.55	Surface Tension of Liquid Fluorocompounds
srf	0.02	N/m	288.05	Surface Tension of Liquid Fluorocompounds
srf	0.02	N/m	313.65	Surface Tension of Liquid Fluorocompounds
srf	0.02	N/m	318.75	Surface Tension of Liquid Fluorocompounds
srf	0.02	N/m	293.35	Surface Tension of Liquid Fluorocompounds
srf	0.02	N/m	298.45	Surface Tension of Liquid Fluorocompounds
srf	0.02	N/m	303.45	Surface Tension of Liquid Fluorocompounds

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	354.70	K	99.10	NIST Webbook
tbrp	354.50 ± 0.50	K	99.10	NIST Webbook

Correlations

Information	Value
Property code	pvap

Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.38550e+01
Coeff. B	-2.57337e+03
Coeff. C	-7.63960e+01
Temperature range (K), min.	266.07
Temperature range (K), max.	377.60

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	9.63466e+01
Coeff. B	-7.45555e+03
Coeff. C	-1.22574e+01
Coeff. D	1.03019e-05
Temperature range (K), min.	278.00
Temperature range (K), max.	516.73

Sources

Surface Tension of Liquid Fluorocompounds:	https://www.doi.org/10.1021/je060199g
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C392563&Units=SI
KDB Vapor Pressure Data:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1665
Properties of Perfluorobenzene near the Critical Point:	https://www.doi.org/10.1007/s10765-006-0092-8
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Viscosities of Liquid Fluorocompounds:	https://www.doi.org/10.1021/je700632z
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
KDB:	https://www.cheric.org/files/research/kdb/mol/mol1665.mol
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
Solubility of Hexafluorobenzene in Aqueous Salt Solutions from (280 to 340) K:	https://www.doi.org/10.1021/je049707h
KDB Pure (Korean Thermophysical Properties Databank):	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1665
Densities and Vapor Pressures of Highly Fluorinated Compounds:	https://www.doi.org/10.1021/je050056e
Reassembling and testing of a high-precision heat capacity drop calorimeter. Heat capacity of some polyphenyls at T = 298.15 K:	https://www.doi.org/10.1016/j.jct.2011.06.010
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

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
ea:	Electron affinity
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
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
kvisc:	Kinematic viscosity
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
pvap:	Vapor pressure
rhoc:	Critical density
rhol:	Liquid Density
rinpol:	Non-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
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
tt:	Triple Point Temperature
vc:	Critical Volume
zc:	Critical Compressibility