Benzene, pentafluoro-

Other names:	1,2,3,4,5-PENTAFLUOROBENZENE
	Pentafluorobenzene
Inchi:	InChI=1S/C6HF5/c7-2-1-3(8)5(10)6(11)4(2)9/h1H
InchiKey:	WACNXHCZHTVBJM-UHFFFAOYSA-N
Formula:	C6HF5
SMILES:	Fc1cc(F)c(F)c(F)c1F
Mol. weight [g/mol]:	168.06
CAS:	363-72-4

Physical Properties

Property code	Value	Unit	Source
af	0.3730		KDB
affp	690.40	kJ/mol	NIST Webbook
basg	662.70	kJ/mol	NIST Webbook
chl	-2557.00 ± 1.40	kJ/mol	NIST Webbook
ea	0.43 ± 0.09	eV	NIST Webbook
ea	0.73 ± 0.08	eV	NIST Webbook
gf	-900.52	kJ/mol	Joback Method
hf	-806.00 ± 1.40	kJ/mol	NIST Webbook
hfl	-842.20 ± 1.40	kJ/mol	NIST Webbook
hfus	19.18	kJ/mol	Joback Method
hvap	36.20 ± 0.20	kJ/mol	NIST Webbook
hvap	36.20	kJ/mol	NIST Webbook
hvap	36.36	kJ/mol	NIST Webbook
hvap	36.39	kJ/mol	NIST Webbook
ie	9.84	eV	NIST Webbook
ie	9.63	eV	NIST Webbook
ie	9.63 ± 0.00	eV	NIST Webbook
ie	9.82	eV	NIST Webbook
ie	9.90	eV	NIST Webbook
ie	9.64	eV	NIST Webbook
ie	9.73	eV	NIST Webbook
log10ws	-3.13		Crippen Method
logp	2.382		Crippen Method
mcvol	80.490	ml/mol	McGowan Method
pc	3531.00 ± 5.00	kPa	NIST Webbook
pc	3470.00	kPa	NIST Webbook

pc	3516.00 ± 10.00	kPa	NIST Webbook
pc	3531.00	kPa	KDB
rhoc	517.64 ± 0.50	kg/m3	NIST Webbook
rinpol	589.00		NIST Webbook
rinpol	594.00		NIST Webbook
rinpol	589.00		NIST Webbook
sl	279.49	J/mol×K	NIST Webbook
sl	275.90	J/mol×K	NIST Webbook
tb	357.75 ± 0.05	K	NIST Webbook
tb	358.89	K	KDB
tb	358.00	K	NIST Webbook
tb	357.50 ± 0.50	K	NIST Webbook
tb	358.90	K	NIST Webbook
tb	358.89 ± 0.00	K	NIST Webbook
tb	358.89 ± 0.01	K	NIST Webbook
tb	358.20	K	NIST Webbook
tc	530.97	K	KDB
tc	531.04	K	Density of Vapor and Liquid Pentafluorobenzene Along the Saturation Line
tc	532.00	K	NIST Webbook
tc	530.80	K	NIST Webbook
tc	530.96 ± 0.05	K	NIST Webbook
tc	531.95 ± 0.05	K	NIST Webbook
tc	530.97 ± 0.03	K	NIST Webbook
tf	225.80	K	KDB
tt	225.83 ± 0.02	K	NIST Webbook
tt	225.67 ± 0.02	K	NIST Webbook
vc	0.324	m3/kmol	KDB
zc	0.2591410		KDB

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	172.20	J/mol×K	490.07	Joback Method
cpg	177.11	J/mol×K	517.69	Joback Method
cpg	150.60	J/mol×K	379.63	Joback Method
cpg	156.29	J/mol×K	407.24	Joback Method
cpg	161.79	J/mol×K	434.85	Joback Method
cpg	167.09	J/mol×K	462.46	Joback Method
cpg	181.83	J/mol×K	545.30	Joback Method
cpl	210.79	J/mol×K	298.15	NIST Webbook

cpl	204.70	J/mol×K	298.15	NIST Webbook
hfust	10.88	kJ/mol	225.70	NIST Webbook
hfust	10.88	kJ/mol	225.70	NIST Webbook
hfust	10.88	kJ/mol	225.67	NIST Webbook
hfust	10.85	kJ/mol	225.83	NIST Webbook
hvapt	32.00	kJ/mol	451.50	NIST Webbook
hvapt	35.70	kJ/mol	328.00	NIST Webbook
hvapt	32.15	kJ/mol	358.90	NIST Webbook
hvapt	33.50	kJ/mol	377.50	NIST Webbook
hvapt	32.60	kJ/mol	436.00	NIST Webbook
hvapt	32.20	kJ/mol	502.00	NIST Webbook
hvapt	34.80	kJ/mol	345.00	NIST Webbook
hvapt	34.78 ± 0.01	kJ/mol	190.00	NIST Webbook
rhol	1453.00	kg/m3	327.60	Liquid-Liquid Equilibria in Binary Mixtures Containing Fluorinated Benzenes and Ionic Liquid 1-Ethyl-3-methylimidazolium Bis(trifluoromethylsulfonyl)imide
rhol	1511.00	kg/m3	296.90	Liquid-Liquid Equilibria in Binary Mixtures Containing Fluorinated Benzenes and Ionic Liquid 1-Ethyl-3-methylimidazolium Bis(trifluoromethylsulfonyl)imide
sfust	48.06	J/mol×K	225.83	NIST Webbook
sfust	48.22	J/mol×K	225.67	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.43600e+01
Coeff. B	-2.94750e+03
Coeff. C	-5.54340e+01
Temperature range (K), min.	264.89
Temperature range (K), max.	381.18

Information	Value

Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	8.99831e+01
Coeff. B	-7.29499e+03
Coeff. C	-1.12510e+01
Coeff. D	8.93524e-06
Temperature range (K), min.	322.00
Temperature range (K), max.	526.82

Sources

Density of Vapor and Liquid Pentafluorobenzene Along the Saturation Line:	https://www.doi.org/10.1007/s10765-010-0886-6
KDB:	https://www.cheric.org/files/research/kdb/mol/mol1666.mol
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C363724&Units=SI
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
KDB Vapor Pressure Data:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1666
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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

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
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
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
tt:	Triple Point Temperature
vc:	Critical Volume
zc:	Critical Compressibility