Benzene, chloropentafluoro-

Other names:	CHLOROPERFLUOROBENZENE
	Chloropentafluorobenzene
	PENTAFLUOROPHENYL CHLORIDE
	Pentafluorochlorobenzene
Inchi:	InChI=1S/C6ClF5/c7-1-2(8)4(10)6(12)5(11)3(1)9
InchiKey:	KGCDGLXSBHJAHZ-UHFFFAOYSA-N
Formula:	C6ClF5
SMILES:	Fc1c(F)c(F)c(Cl)c(F)c1F
Mol. weight [g/mol]:	202.51
CAS:	344-07-0

Physical Properties

Property code	Value	Unit	Source
af	0.4000		KDB
chl	-2428.70 ± 2.00	kJ/mol	NIST Webbook
ea	0.82 ± 0.11	eV	NIST Webbook
ea	0.75 ± 0.08	eV	NIST Webbook
gf	-922.08	kJ/mol	Joback Method
hf	-809.60 ± 2.00	kJ/mol	NIST Webbook
hfl	-850.40 ± 2.20	kJ/mol	NIST Webbook
hfus	22.99	kJ/mol	Joback Method
hvap	41.10	kJ/mol	NIST Webbook
hvap	40.80 ± 0.40	kJ/mol	NIST Webbook
hvap	41.30	kJ/mol	NIST Webbook
ie	9.72 ± 0.14	eV	NIST Webbook
ie	9.50	eV	NIST Webbook
ie	10.40 ± 0.10	eV	NIST Webbook
ie	9.72 ± 0.02	eV	NIST Webbook
ie	9.94	eV	NIST Webbook
log10ws	-3.81		Crippen Method
logp	3.035		Crippen Method
mcvol	92.730	ml/mol	McGowan Method
pc	3238.00	kPa	KDB
pc	3190.00	kPa	NIST Webbook
rhoc	538.88 ± 0.53	kg/m3	NIST Webbook
rinpol	748.00		NIST Webbook
sl	303.59	J/mol×K	NIST Webbook

sl	300.70	J/mol×K	NIST Webbook
tb	391.11	K	KDB
tb	391.20	K	NIST Webbook
tb	390.00	K	NIST Webbook
tc	570.81 ± 0.05	K	NIST Webbook
tc	569.90	K	NIST Webbook
tc	571.00	K	NIST Webbook
tc	570.81	K	KDB
tf	279.27	K	Joback Method
tt	257.49 ± 0.02	K	NIST Webbook
tt	257.29 ± 0.02	K	NIST Webbook
vc	0.376	m3/kmol	KDB
zc	0.2565290		KDB

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	199.06	J/mol×K	596.57	Joback Method
cpg	190.52	J/mol×K	538.39	Joback Method
cpg	194.88	J/mol×K	567.48	Joback Method
cpg	171.33	J/mol×K	422.04	Joback Method
cpg	176.39	J/mol×K	451.13	Joback Method
cpg	181.27	J/mol×K	480.22	Joback Method
cpg	185.98	J/mol×K	509.31	Joback Method
cpl	221.40	J/mol×K	298.15	NIST Webbook
cpl	223.17	J/mol×K	298.15	NIST Webbook
hfust	3.64	kJ/mol	191.00	NIST Webbook
hfust	0.98	kJ/mol	245.00	NIST Webbook
hfust	8.36	kJ/mol	257.50	NIST Webbook
hfust	8.36	kJ/mol	257.50	NIST Webbook
hvapt	35.20	kJ/mol	475.00	NIST Webbook
hvapt	34.80 ± 0.10	kJ/mol	391.00	NIST Webbook
hvapt	34.76 ± 0.01	kJ/mol	391.10	NIST Webbook
hvapt	34.76	kJ/mol	391.20	NIST Webbook
hvapt	37.70	kJ/mol	375.00	NIST Webbook
hvapt	40.00	kJ/mol	362.00	NIST Webbook
hvapt	37.70 ± 0.10	kJ/mol	349.00	NIST Webbook
hvapt	36.40 ± 0.10	kJ/mol	369.00	NIST Webbook
sfust	32.45	J/mol×K	257.50	NIST Webbook
sfust	4.01	J/mol×K	245.00	NIST Webbook
sfust	19.04	J/mol×K	191.00	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	395.70	K	100.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.44250e+01
Coeff. B	-3.27746e+03
Coeff. C	-5.69020e+01
Temperature range (K), min.	288.73
Temperature range (K), max.	416.53

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	9.08383e+01
Coeff. B	-7.91458e+03
Coeff. C	-1.12535e+01
Coeff. D	7.77116e-06
Temperature range (K), min.	308.15
Temperature range (K), max.	565.76

Sources

KDB Vapor Pressure Data: https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1661

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

KDB: https://www.cheric.org/files/research/kdb/mol/mol1661.mol

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C344070&Units=SI
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

Legend

af:	Acentric Factor
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
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
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
tt:	Triple Point Temperature
vc:	Critical Volume
zc:	Critical Compressibility