Benzene, pentafluoromethyl-

Other names:	2,3,4,5,6-Pentafluoro-1-methylbenzene
	2,3,4,5,6-Pentafluorotoluene
	Methyl pentafluorobenzene
	PENTAFLUOROMETHYLBENZENE
	Pentafluorotoluene
	Toluene, 2,3,4,5,6-pentafluoro-
Inchi:	InChI=1S/C7H3F5/c1-2-3(8)5(10)7(12)6(11)4(2)9/h1H3
InchiKey:	SXPRVMIZFRCAGC-UHFFFAOYSA-N
Formula:	C7H3F5
SMILES:	Cc1c(F)c(F)c(F)c(F)c1F
Mol. weight [g/mol]:	182.09
CAS:	771-56-2

Physical Properties

Property code	Value	Unit	Source
af	0.4150		KDB
chl	-3194.40 ± 1.50	kJ/mol	NIST Webbook
gf	-901.73	kJ/mol	Joback Method
hf	-843.30 ± 1.50	kJ/mol	NIST Webbook
hfl	-884.20 ± 1.50	kJ/mol	NIST Webbook
hfus	21.38	kJ/mol	Joback Method
hvap	41.13	kJ/mol	NIST Webbook
hvap	40.90 ± 0.40	kJ/mol	NIST Webbook
hvap	41.20	kJ/mol	NIST Webbook
ie	9.40	eV	NIST Webbook
ie	9.81	eV	NIST Webbook
ie	9.40	eV	NIST Webbook
ie	9.60 ± 0.10	eV	NIST Webbook
log10ws	-3.61		Crippen Method
logp	2.691		Crippen Method
mcvol	94.580	ml/mol	McGowan Method
pc	3126.00	kPa	KDB
rhoc	473.44 ± 0.47	kg/m3	NIST Webbook
sl	310.87	J/mol×K	NIST Webbook
sl	306.40	J/mol×K	NIST Webbook
tb	390.60	K	NIST Webbook
tb	390.60	K	KDB

tb	390.00	K	NIST Webbook
tb	390.20	K	NIST Webbook
tc	566.52 ± 0.05	K	NIST Webbook
tc	566.52	K	KDB
tc	548.60	K	NIST Webbook
tf	243.30	K	KDB
tt	243.35 ± 0.02	K	NIST Webbook
tt	243.70 ± 0.20	K	NIST Webbook
vc	0.384	m3/kmol	KDB
zc	0.2548400		KDB

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	185.43	J/mol×K	407.49	Joback Method
cpg	192.04	J/mol×K	435.26	Joback Method
cpg	198.45	J/mol×K	463.02	Joback Method
cpg	204.65	J/mol×K	490.79	Joback Method
cpg	210.65	J/mol×K	518.55	Joback Method
cpg	216.44	J/mol×K	546.32	Joback Method
cpg	222.03	J/mol×K	574.08	Joback Method
cpl	231.12	J/mol×K	298.15	NIST Webbook
cpl	225.80	J/mol×K	298.15	NIST Webbook
hfust	13.28	kJ/mol	243.70	NIST Webbook
hfust	13.28	kJ/mol	243.70	NIST Webbook
hvapt	34.75	kJ/mol	390.60	NIST Webbook
hvapt	36.10	kJ/mol	463.00	NIST Webbook
hvapt	34.90	kJ/mol	528.50	NIST Webbook
hvapt	39.90	kJ/mol	364.00	NIST Webbook
sfust	54.49	J/mol×K	243.70	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.39378e+01
Coeff. B	-3.07019e+03

Coeff. C	-6.36160e+01
Temperature range (K), min.	288.54
Temperature range (K), max.	419.53

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	7.89485e+01
Coeff. B	-7.41141e+03
Coeff. C	-9.43421e+00
Coeff. D	6.17295e-06
Temperature range (K), min.	312.15
Temperature range (K), max.	566.15

Sources

KDB Vapor Pressure Data: https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1689

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/mol1689.mol

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C771562&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

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
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