Benzene, 1,2,3,4-tetrafluoro-

Other names: 1,2,3,4-Tetrafluorobenzene
2,3,4,5-Tetrafluorobenzene
Inchi: InChI=1S/C6H2F4/c7-3-1-2-4(8)6(10)5(3)9/h1-2H
InchiKey: SOZFIIXUNAKEJP-UHFFFAOYSA-N
Formula: C6H2F4
SMILES: Fc1ccc(F)c(F)c1F
Mol. weight [g/mol]: 150.07
CAS: 551-62-2

Physical Properties

Property code	Value	Unit	Source
af	0.3440		KDB
affp	700.40	kJ/mol	NIST Webbook
basg	672.70	kJ/mol	NIST Webbook
gf	-696.08	kJ/mol	Joback Method
hf	-749.49	kJ/mol	Joback Method
hfus	16.49	kJ/mol	Joback Method
hvap	37.50	kJ/mol	NIST Webbook
ie	9.57 ± 0.03	eV	NIST Webbook
ie	9.60	eV	NIST Webbook
ie	9.53 ± 0.00	eV	NIST Webbook
ie	9.61	eV	NIST Webbook
ie	9.56	eV	NIST Webbook
log10ws	-2.80		Crippen Method
logp	2.243		Crippen Method
mcvol	78.720	ml/mol	McGowan Method
pc	3791.00	kPa	KDB
pc	3791.00 ± 4.00	kPa	NIST Webbook
rhoc	479.64 ± 0.47	kg/m3	NIST Webbook
sl	256.10	J/mol×K	NIST Webbook
tb	368.20	K	NIST Webbook
tb	367.51	K	KDB
tb	366.70	K	NIST Webbook
tb	368.00	K	NIST Webbook
tc	550.83	K	KDB
tc	550.83 ± 0.20	K	NIST Webbook
tc	550.83 ± 0.05	K	NIST Webbook

tf	223.72	K	Joback Method
tt	233.26 ± 0.02	K	NIST Webbook
tt	231.25 ± 0.02	K	NIST Webbook
vc	0.313	m3/kmol	KDB
zc	0.2590860		KDB

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	141.11	J/mol×K	375.38	Joback Method
cpg	147.59	J/mol×K	404.29	Joback Method
cpg	153.81	J/mol×K	433.20	Joback Method
cpg	159.77	J/mol×K	462.11	Joback Method
cpg	165.47	J/mol×K	491.02	Joback Method
cpg	170.93	J/mol×K	519.93	Joback Method
cpg	176.14	J/mol×K	548.84	Joback Method
cpl	189.90	J/mol×K	298.15	NIST Webbook
hfust	10.93	kJ/mol	233.30	NIST Webbook
hfust	10.93	kJ/mol	233.30	NIST Webbook
hvapt	36.80	kJ/mol	346.00	NIST Webbook
hvapt	37.00	kJ/mol	301.00	NIST Webbook
rhol	1408.00	kg/m3	296.40	Liquid-Liquid Equilibria in Binary Mixtures Containing Fluorinated Benzenes and Ionic Liquid 1-Ethyl-3-methylimidazolium Bis(trifluoromethylsulfonyl)imide
rhol	1360.00	kg/m3	327.40	Liquid-Liquid Equilibria in Binary Mixtures Containing Fluorinated Benzenes and Ionic Liquid 1-Ethyl-3-methylimidazolium Bis(trifluoromethylsulfonyl)imide

Correlations

Information	Value

Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.80331e+01
Coeff. B	-3.77649e+03
Coeff. C	-5.78220e+01
Temperature range (K), min.	270.64
Temperature range (K), max.	354.68

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	7.10221e+01
Coeff. B	-6.63473e+03
Coeff. C	-8.31885e+00
Coeff. D	5.79106e-06
Temperature range (K), min.	279.15
Temperature range (K), max.	546.00

Sources

The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
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/mol1667.mol
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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C551622&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
KDB Vapor Pressure Data:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1667

Legend

af:	Acentric Factor
affp:	Proton affinity
basg:	Gas basicity
cpg:	Ideal gas heat capacity
cpl:	Liquid phase heat capacity

gf:	Standard Gibbs free energy of formation
hf:	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
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