Benzene, 1,2,4,5-tetrafluoro-

Other names: 1,2,4,5-Tetrafluorobenzene
2,3,5,6-Tetrafluorobenzene
Inchi: InChI=1S/C6H2F4/c7-3-1-4(8)6(10)2-5(3)9/h1-2H
InchiKey: SDXUIOOHCIQXRP-UHFFFAOYSA-N
Formula: C6H2F4
SMILES: Fc1cc(F)c(F)cc1F
Mol. weight [g/mol]: 150.07
CAS: 327-54-8

Physical Properties

Property code	Value	Unit	Source
af	0.3550		KDB
affp	746.50	kJ/mol	NIST Webbook
basg	718.80	kJ/mol	NIST Webbook
chl	-2679.00 ± 1.70	kJ/mol	NIST Webbook
gf	-696.08	kJ/mol	Joback Method
hf	-646.80 ± 3.40	kJ/mol	NIST Webbook
hfl	-683.80 ± 3.20	kJ/mol	NIST Webbook
hfus	16.49	kJ/mol	Joback Method
hvap	37.20	kJ/mol	NIST Webbook
hvap	37.11	kJ/mol	NIST Webbook
ie	9.20	eV	NIST Webbook
ie	9.35 ± 0.00	eV	NIST Webbook
ie	9.33 ± 0.07	eV	NIST Webbook
ie	9.36	eV	NIST Webbook
ie	9.39	eV	NIST Webbook
log10ws	-2.38		Aqueous Solubility Prediction Method
logp	2.243		Crippen Method
mcvol	78.720	ml/mol	McGowan Method
pc	3801.00 ± 6.00	kPa	NIST Webbook
pc	3801.00	kPa	KDB
rinpol	604.00		NIST Webbook
sl	250.40	J/mol×K	NIST Webbook
tb	363.00	K	NIST Webbook
tb	362.70	K	NIST Webbook
tb	363.41	K	KDB

tc	543.35	K	KDB
tc	543.35 ± 0.20	K	NIST Webbook
tf	277.40	K	Aqueous Solubility Prediction Method
tf	277.60	K	KDB
tt	277.03 ± 0.02	K	NIST Webbook
vc	0.336	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	147.59	J/mol×K	404.29	Joback Method
cpg	153.81	J/mol×K	433.20	Joback Method
cpg	176.14	J/mol×K	548.84	Joback Method
cpg	170.93	J/mol×K	519.93	Joback Method
cpg	165.47	J/mol×K	491.02	Joback Method
cpg	159.77	J/mol×K	462.11	Joback Method
cpg	141.11	J/mol×K	375.38	Joback Method
cpl	192.20	J/mol×K	298.15	NIST Webbook
hfust	15.05	kJ/mol	277.00	NIST Webbook
hfust	15.05	kJ/mol	277.00	NIST Webbook
hfust	15.05	kJ/mol	277.03	NIST Webbook
hvapt	36.80	kJ/mol	341.50	NIST Webbook
hvapt	32.60	kJ/mol	515.50	NIST Webbook
hvapt	33.10	kJ/mol	439.00	NIST Webbook
rhol	1370.00	kg/m3	327.40	Liquid-Liquid Equilibria in Binary Mixtures Containing Fluorinated Benzenes and Ionic Liquid 1-Ethyl-3-methylimidazolium Bis(trifluoromethylsulfonyl)imide
rhol	1421.00	kg/m3	296.70	Liquid-Liquid Equilibria in Binary Mixtures Containing Fluorinated Benzenes and Ionic Liquid 1-Ethyl-3-methylimidazolium Bis(trifluoromethylsulfonyl)imide
sfust	54.33	J/mol×K	277.03	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	2.16950e+01
Coeff. B	-5.07479e+03
Coeff. C	-4.21610e+01
Temperature range (K), min.	279.22
Temperature range (K), max.	351.91

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	8.90733e+01
Coeff. B	-7.34595e+03
Coeff. C	-1.10868e+01
Coeff. D	8.49380e-06
Temperature range (K), min.	293.15
Temperature range (K), max.	543.00

Sources

The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
KDB:	https://www.cheric.org/files/research/kdb/mol/mol1669.mol
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C327548&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
KDB Vapor Pressure Data:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1669

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
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
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

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https://www.chemeo.com/cid/54-763-5/Benzene-1-2-4-5-tetrafluoro.pdf
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