Benzene, 1,4-difluoro-

Other names:	1,4-DIFLUOROBENZENE
	Benzene, p-difluoro-
	p-Difluorobenzene
	para-Difluorobenzene
Inchi:	InChI=1S/C6H4F2/c7-5-1-2-6(8)4-3-5/h1-4H
InchiKey:	QUGUFLJIAFISSW-UHFFFAOYSA-N
Formula:	C6H4F2
SMILES:	Fc1ccc(F)cc1
Mol. weight [g/mol]:	114.09
CAS:	540-36-3

Physical Properties

Property code	Value	Unit	Source
af	0.2990		KDB
affp	718.70	kJ/mol	NIST Webbook
basg	692.80	kJ/mol	NIST Webbook
chl	-2954.00	kJ/mol	NIST Webbook
chl	-2948.40 ± 0.54	kJ/mol	NIST Webbook
gf	-253.00	kJ/mol	KDB
hf	-306.70 ± 1.00	kJ/mol	NIST Webbook
hf	-307.40	kJ/mol	KDB
hfl	-342.30 ± 1.00	kJ/mol	NIST Webbook
hfus	11.11	kJ/mol	Joback Method
hvap	35.68	kJ/mol	NIST Webbook
hvap	35.60 ± 0.20	kJ/mol	NIST Webbook
hvap	35.80	kJ/mol	NIST Webbook
hvap	35.62	kJ/mol	NIST Webbook
ie	9.40 ± 0.03	eV	NIST Webbook
ie	9.15	eV	NIST Webbook
ie	9.40	eV	NIST Webbook
ie	9.15 ± 0.06	eV	NIST Webbook
ie	9.18	eV	NIST Webbook
ie	9.14 ± 0.00	eV	NIST Webbook
ie	9.14	eV	NIST Webbook
ie	9.16 ± 0.00	eV	NIST Webbook
ie	9.16 ± 0.00	eV	NIST Webbook
ie	9.16 ± 0.00	eV	NIST Webbook

ie	9.29	eV	NIST Webbook
ie	9.15	eV	NIST Webbook
log10ws	-1.97		Estimated Solubility Method
log10ws	-1.97		Aqueous Solubility Prediction Method
logp	1.965		Crippen Method
mcvol	75.180	ml/mol	McGowan Method
pc	4400.00	kPa	KDB
rinpol	665.00		NIST Webbook
rinpol	666.00		NIST Webbook
rinpol	666.00		NIST Webbook
tb	362.20	K	NIST Webbook
tb	362.00	K	NIST Webbook
tb	362.00 ± 3.00	K	NIST Webbook
tb	360.50 ± 0.50	K	NIST Webbook
tb	362.00	K	KDB
tc	556.00	K	KDB
tf	249.60 ± 0.08	K	NIST Webbook
tf	260.00	K	KDB
vc	0.299	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	145.31	J/mol×K	462.36	Joback Method
cpg	152.37	J/mol×K	494.18	Joback Method
cpg	159.04	J/mol×K	526.01	Joback Method
cpg	121.64	J/mol×K	366.88	Joback Method
cpg	129.96	J/mol×K	398.71	Joback Method
cpg	137.84	J/mol×K	430.53	Joback Method
cpg	165.34	J/mol×K	557.84	Joback Method
cpl	159.10	J/mol×K	298.15	NIST Webbook
cpl	157.50	J/mol×K	298.15	NIST Webbook
hvapt	31.77	kJ/mol	362.00	NIST Webbook
rhol	1146.00	kg/m3	296.10	Liquid-Liquid Equilibria in Binary Mixtures Containing Fluorinated Benzenes and Ionic Liquid 1-Ethyl-3-methylimidazolium Bis(trifluoromethylsulfonyl)imide

rhol	1110.00	kg/m3	327.20	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	1.45561e+01
Coeff. B	-3.16523e+03
Coeff. C	-4.36940e+01
Temperature range (K), min.	260.16
Temperature range (K), max.	386.08

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	7.10061e+01
Coeff. B	-6.47535e+03
Coeff. C	-8.37270e+00
Coeff. D	6.31383e-06
Temperature range (K), min.	300.15
Temperature range (K), max.	556.00

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Estimated Solubility Method:	http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
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
KDB:	https://www.cheric.org/files/research/kdb/mol/mol1682.mol
KDB Vapor Pressure Data:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1682

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C540363&Units=SI
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

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