Benzene, 1,3-difluoro-

Other names:	1,3-DIFLUOROBENZENE
	Benzene, m-difluoro-
	m-Difluorobenzene
	meta-Difluorobenzene
Inchi:	InChI=1S/C6H4F2/c7-5-2-1-3-6(8)4-5/h1-4H
InchiKey:	UEMGWPRHOOEKTA-UHFFFAOYSA-N
Formula:	C6H4F2
SMILES:	Fc1cccc(F)c1
Mol. weight [g/mol]:	114.09
CAS:	372-18-9

Physical Properties

Property code	Value	Unit	Source
affp	749.70	kJ/mol	NIST Webbook
basg	722.00	kJ/mol	NIST Webbook
chl	-2946.70 ± 0.71	kJ/mol	NIST Webbook
gf	-287.20	kJ/mol	Joback Method
hf	-309.20 ± 1.00	kJ/mol	NIST Webbook
hfl	-343.90 ± 1.00	kJ/mol	NIST Webbook
hfus	11.11	kJ/mol	Joback Method
hvap	34.70 ± 0.20	kJ/mol	NIST Webbook
hvap	34.69	kJ/mol	NIST Webbook
hvap	34.55	kJ/mol	NIST Webbook
hvap	34.60	kJ/mol	NIST Webbook
ie	9.32	eV	NIST Webbook
ie	9.33 ± 0.02	eV	NIST Webbook
ie	9.35	eV	NIST Webbook
ie	9.60 ± 0.03	eV	NIST Webbook
ie	9.78 ± 0.02	eV	NIST Webbook
ie	9.33 ± 0.00	eV	NIST Webbook
ie	9.20	eV	NIST Webbook
log10ws	-2.00		Estimated Solubility Method
log10ws	-2.00		Aqueous Solubility Prediction Method
logp	1.965		Crippen Method
mcvol	75.180	ml/mol	McGowan Method
pc	4067.32	kPa	Joback Method

rinpol	644.00		NIST Webbook
rinpol	641.70		NIST Webbook
rinpol	644.00		NIST Webbook
sl	223.84	J/mol×K	NIST Webbook
tb	356.20	K	NIST Webbook
tb	355.70	K	NIST Webbook
tb	355.00 ± 1.00	K	NIST Webbook
tc	557.84	K	Joback Method
tf	197.50	K	Joback Method
tt	204.03	K	KDB
tt	204.03 ± 0.02	K	NIST Webbook
vc	0.299	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	121.64	J/mol×K	366.88	Joback Method
cpg	129.96	J/mol×K	398.71	Joback Method
cpg	165.34	J/mol×K	557.84	Joback Method
cpg	159.04	J/mol×K	526.01	Joback Method
cpg	152.37	J/mol×K	494.18	Joback Method
cpg	145.31	J/mol×K	462.36	Joback Method
cpg	137.84	J/mol×K	430.53	Joback Method
cpl	159.11	J/mol×K	298.15	NIST Webbook
cpl	157.50	J/mol×K	298.15	NIST Webbook
hfust	0.83	kJ/mol	186.80	NIST Webbook
hfust	8.58	kJ/mol	204.00	NIST Webbook
hfust	8.58	kJ/mol	204.00	NIST Webbook
hvapt	31.10	kJ/mol	355.70	NIST Webbook
rhol	1094.00	kg/m3	330.60	Liquid-Liquid Equilibria in Binary Mixtures Containing Fluorinated Benzenes and Ionic Liquid 1-Ethyl-3-methylimidazolium Bis(trifluoromethylsulfonyl)imide

rhol	1139.00	kg/m3	296.20	Liquid-Liquid Equilibria in Binary Mixtures Containing Fluorinated Benzenes and Ionic Liquid 1-Ethyl-3-methylimidazolium Bis(trifluoromethylsulfonyl)imide
sfust	42.05	J/mol×K	204.00	NIST Webbook
sfust	4.43	J/mol×K	186.80	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.55597e+01
Coeff. B	-3.42581e+03
Coeff. C	-4.18950e+01
Temperature range (K), min.	266.21
Temperature range (K), max.	376.18

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	9.46186e+01
Coeff. B	-7.08505e+03
Coeff. C	-1.22131e+01
Coeff. D	1.19919e-05
Temperature range (K), min.	309.15
Temperature range (K), max.	552.94

Sources

KDB Vapor Pressure Data: https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1681

Estimated Solubility Method: http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt

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

Aqueous Solubility Prediction Method: http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C372189&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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/mol1681.mol

Legend

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