Benzene, 1,2-difluoro-

Other names:	1,2-DIFLUOROBENZENE Benzene, o-difluoro- benzene, 1,2-difluror- o-Difluorobenzene ortho-Difluorobenzene
Inchi:	InChI=1S/C6H4F2/c7-5-3-1-2-4-6(5)8/h1-4H
InchiKey:	GOYDNIKZWGIXJT-UHFFFAOYSA-N
Formula:	C6H4F2
SMILES:	Fc1ccccc1F
Mol. weight [g/mol]:	114.09
CAS:	367-11-3

Physical Properties

Property code	Value	Unit	Source
affp	731.20	kJ/mol	NIST Webbook
basg	703.50	kJ/mol	NIST Webbook
chl	-2960.70 ± 0.54	kJ/mol	NIST Webbook
gf	-287.20	kJ/mol	Joback Method
hf	-283.00 ± 0.92	kJ/mol	NIST Webbook
hfl	-319.20 ± 0.92	kJ/mol	NIST Webbook
hfus	11.11	kJ/mol	Joback Method
hvap	36.24	kJ/mol	NIST Webbook
hvap	36.20	kJ/mol	NIST Webbook
hvap	36.20	kJ/mol	NIST Webbook
hvap	36.20 ± 0.08	kJ/mol	NIST Webbook
ie	9.60 ± 0.03	eV	NIST Webbook
ie	9.30	eV	NIST Webbook
ie	9.31	eV	NIST Webbook
ie	9.74 ± 0.02	eV	NIST Webbook
ie	9.30	eV	NIST Webbook
ie	9.28 ± 0.01	eV	NIST Webbook
ie	9.29 ± 0.01	eV	NIST Webbook
log10ws	-2.13		Crippen Method
logp	1.965		Crippen Method
mcvol	75.180	ml/mol	McGowan Method
pc	4067.32	kPa	Joback Method
rinpol	674.40		NIST Webbook

rinpol	681.00		NIST Webbook
rinpol	674.40		NIST Webbook
rinpol	675.00		NIST Webbook
sl	222.59	J/mol×K	NIST Webbook
tb	367.10	K	NIST Webbook
tb	364.50 ± 0.50	K	NIST Webbook
tb	365.20	K	NIST Webbook
tc	557.30	K	NIST Webbook
tf	197.50	K	Joback Method
tt	226.01 ± 0.01	K	NIST Webbook
vc	0.299	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	165.34	J/mol×K	557.84	Joback Method
cpg	121.64	J/mol×K	366.88	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
cpg	129.96	J/mol×K	398.71	Joback Method
cpl	159.40	J/mol×K	298.15	NIST Webbook
cpl	159.03	J/mol×K	298.15	NIST Webbook
hfust	11.05	kJ/mol	226.00	NIST Webbook
hfust	11.05	kJ/mol	226.00	NIST Webbook
hfust	11.05	kJ/mol	226.01	NIST Webbook
hvapt	32.20 ± 0.10	kJ/mol	367.00	NIST Webbook
hvapt	34.60 ± 0.10	kJ/mol	327.00	NIST Webbook
hvapt	35.50	kJ/mol	353.50	NIST Webbook
hvapt	32.21	kJ/mol	367.10	NIST Webbook
hvapt	33.50 ± 0.10	kJ/mol	345.00	NIST Webbook
rhol	1117.00	kg/m3	331.10	Liquid-Liquid Equilibria in Binary Mixtures Containing Fluorinated Benzenes and Ionic Liquid 1-Ethyl-3-methylimidazolium Bis(trifluoromethylsulfonyl)imide

rhol	1156.00	kg/m3	296.20	Liquid-Liquid Equilibria in Binary Mixtures Containing Fluorinated Benzenes and Ionic Liquid 1-Ethyl-3-methylimidazolium Bis(trifluoromethylsulfonyl)imide
sfust	48.87	J/mol×K	226.01	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	364.70	K	100.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.42556e+01
Coeff. B	-2.97732e+03
Coeff. C	-5.62610e+01
Temperature range (K), min.	269.41
Temperature range (K), max.	389.14

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	7.47430e+01
Coeff. B	-6.68596e+03
Coeff. C	-8.94050e+00
Coeff. D	6.59509e-06
Temperature range (K), min.	304.15
Temperature range (K), max.	405.15

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C367113&Units=SI
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
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=1680
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/mol1680.mol
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature

tf:	Normal melting (fusion) point
tt:	Triple Point Temperature
vc:	Critical Volume

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