Benzene, 1-bromo-2-fluoro-

Other names:	1,2-Fluorobromobenzene
	1-Bromo-2-fluorobenzene
	1-Fluoro-2-bromobenzene
	2-Bromfluorbenzen
	2-Bromofluorobenzene
	2-Fluorobromobenzene
	2-Fluorophenyl bromide
	Benzene, 1-fluoro-2-bromo-
	NSC 59696
	o-Bromofluorobenzene
	o-Fluorobromobenzene
Inchi:	InChI=1S/C6H4BrF/c7-5-3-1-2-4-6(5)8/h1-4H
InchiKey:	IPWBFGUBXWMIPR-UHFFFAOYSA-N
Formula:	C6H4BrF
SMILES:	Fc1ccccc1Br
Mol. weight [g/mol]:	175.00
CAS:	1072-85-1

Physical Properties

Property code	Value	Unit	Source
gf	-78.07	kJ/mol	Joback Method
hf	-111.89	kJ/mol	Joback Method
hfus	13.31	kJ/mol	Joback Method
hvap	37.51	kJ/mol	Joback Method
ie	9.11 ± 0.02	eV	NIST Webbook
ie	9.14	eV	NIST Webbook
log10ws	-2.70		Aqueous Solubility Prediction Method
log10ws	-2.70		Estimated Solubility Method
logp	2.588		Crippen Method
mcvol	90.910	ml/mol	McGowan Method
pc	4730.11	kPa	Joback Method
rinpol	959.60		NIST Webbook
rinpol	934.00		NIST Webbook
rinpol	934.00		NIST Webbook
rinpol	959.60		NIST Webbook

tb	429.00	K	NIST Webbook
tc	657.79	K	Joback Method
tf	256.71	K	Joback Method
vc	0.344	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	144.15	J/mol×K	433.77	Joback Method
cpg	152.60	J/mol×K	471.11	Joback Method
cpg	160.46	J/mol×K	508.44	Joback Method
cpg	167.76	J/mol×K	545.78	Joback Method
cpg	174.52	J/mol×K	583.12	Joback Method
cpg	180.79	J/mol×K	620.45	Joback Method
cpg	186.59	J/mol×K	657.79	Joback Method
hvapt	47.00	kJ/mol	298.15	Vaporization enthalpies of a series of the halogen-substituted fluorobenzenes

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Vaporization enthalpies of a series of the halogen-substituted fluorobenzenes:	https://www.doi.org/10.1016/j.fluid.2014.12.023
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1072851&Units=SI

Legend

cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume