Benzene, 1-fluoro-4-iodo-

Other names:	1,4-fluoroiodobenzene
	1-Fluoro-4-iodobenzene
	4-Fluoroiodobenzene
	4-Iodofluorobenzene
	p-Fluoroiodobenzene
	p-Iodofluorobenzene
Inchi:	InChI=1S/C6H4FI/c7-5-1-3-6(8)4-2-5/h1-4H
InchiKey:	KGNQDBQYEBMPFZ-UHFFFAOYSA-N
Formula:	C6H4FI
SMILES:	Fc1ccc(I)cc1
Mol. weight [g/mol]:	222.00
CAS:	352-34-1

Physical Properties

Property code	Value	Unit	Source
gf	-34.27	kJ/mol	Joback Method
hf	-61.35	kJ/mol	Joback Method
hfus	12.43	kJ/mol	Joback Method
hvap	40.44	kJ/mol	Joback Method
log10ws	-3.13		Aqueous Solubility Prediction Method
logp	2.430		Crippen Method
mcvol	99.230	ml/mol	McGowan Method
pc	4189.32	kPa	Joback Method
tb	456.20	K	NIST Webbook
tb	456.00 ± 1.00	K	NIST Webbook
tc	704.26	K	Joback Method
tf	249.65	K	Aqueous Solubility Prediction Method
vc	0.369	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source

cpg	152.63	J/mol×K	460.75	Joback Method
cpg	161.13	J/mol×K	501.33	Joback Method
cpg	168.95	J/mol×K	541.92	Joback Method
cpg	176.13	J/mol×K	582.50	Joback Method
cpg	182.73	J/mol×K	623.09	Joback Method
cpg	188.79	J/mol×K	663.67	Joback Method
cpg	194.34	J/mol×K	704.26	Joback Method
hvapt	49.50	kJ/mol	298.15	Vaporization enthalpies of a series of the halogen-substituted fluorobenzenes

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C352341&Units=SI
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

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
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume