1-FLUORO-3-IODOBENZENE

Other names:	1,3-fluoroiodobenzene
	3-Fluoroiodobenzene
	3-Iodofluorobenzene
	benzene, 1-fluoro-3-iodo-
	m-Fluorobenzene
	m-Fluoroiodobenzene
	m-Iodofluorobenzene
Inchi:	InChI=1S/C6H4FI/c7-5-2-1-3-6(8)4-5/h1-4H
InchiKey:	VSKSBSORLCDRHS-UHFFFAOYSA-N
Formula:	C6H4FI
SMILES:	Fc1cccc(I)c1
Mol. weight [g/mol]:	222.00

Physical Properties

Property code	Value	Unit	Source
af	0.2700		Cheméo Relay (1.0)
gf	-34.27	kJ/mol	Joback Method
hf	-10.34	kJ/mol	Cheméo Relay (1.0)
hfus	12.43	kJ/mol	Joback Method
hvap	50.23	kJ/mol	Cheméo Relay (1.0)
ie	8.83	eV	Cheméo Relay (1.0)
log10ws	-2.97		Cheméo Relay (1.0)
logp	2.430		Crippen Method
mcvol	99.230	ml/mol	McGowan Method
pc	4189.32	kPa	Joback Method
tb	453.27	K	Cheméo Relay (1.0)
tc	703.10	K	Cheméo Relay (1.0)
tf	231.39	K	Cheméo Relay (1.0)
vc	0.348	m3/kmol	Cheméo Relay (1.0)

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	48.60	kJ/mol	298.15	Vaporization enthalpies of a series of the halogen-substituted fluorobenzenes

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	350.70	K	2.50	NIST Webbook
tbrp	350.50 ± 0.50	K	2.50	NIST Webbook

Sources

Joback Method: https://en.wikipedia.org/wiki/Joback_method

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

Vaporization enthalpies of a series of the halogen-substituted fluorobenzenes: https://www.doi.org/10.1016/j.fluid.2014.12.023

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C1121864&Units=SI

Legend

af: Acentric Factor

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