Benzene, 1-fluoro-3-iodo-

Other names:	1,3-fluoroiodobenzene
	1-fluoro-3-iodobenzene
	3-Fluoroiodobenzene
	3-Iodofluorobenzene
	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
CAS:	1121-86-4

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	-2.95		Crippen Method
logp	2.430		Crippen Method
mcvol	99.230	ml/mol	McGowan Method
pc	4189.32	kPa	Joback Method
tb	460.75	K	Joback Method
tc	704.26	K	Joback Method
tf	254.97	K	Joback 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	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

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1121864&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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

Latest version available from:

https://www.chemeo.com/cid/81-014-6/Benzene-1-fluoro-3-iodo.pdf

Generated by Cheméo on 2024-10-12 08:33:06.305920934 +0000 UTC m=+3302848.942890183.

Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.