Benzene, pentafluoroiodo-

Other names:	Iodopentafluorobenzene
	Pentafluoroiodobenzene
	Pentafluorophenyl iodide
	Iodoperfluorobenzene
	2,3,4,5,6-Pentafluoroiodobenzene
	Perfluoroiodobenzene
	1,2,3,4,5-Pentafluoro-6-iodo-benzene
Inchi:	InChI=1S/C6F5I/c7-1-2(8)4(10)6(12)5(11)3(1)9
InchiKey:	OPYHNLNYCRZOGY-UHFFFAOYSA-N
Formula:	C6F5I
SMILES:	Fc1c(F)c(F)c(I)c(F)c1F
Mol. weight [g/mol]:	293.96
CAS:	827-15-6

Physical Properties

Property code	Value	Unit	Source
chl	-2201.00 ± 13.00	kJ/mol	NIST Webbook
ea	1.41 ± 0.11	eV	NIST Webbook
gf	-852.03	kJ/mol	Joback Method
hf	-549.00 ± 13.00	kJ/mol	NIST Webbook
hfus	23.20	kJ/mol	Joback Method
hvap	57.90 ± 0.20	kJ/mol	NIST Webbook
ie	9.54	eV	NIST Webbook
ie	9.54	eV	NIST Webbook
ie	9.50 ± 0.10	eV	NIST Webbook
log10ws	-4.28		Crippen Method
logp	2.987		Crippen Method
mcvol	106.310	ml/mol	McGowan Method
pc	3138.51	kPa	Joback Method
tb	439.00	K	NIST Webbook
tb	434.20	K	NIST Webbook
tc	677.68	K	Joback Method
tf	307.41	K	Joback Method
vc	0.442	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	184.49	J/mol×K	477.75	Joback Method
cpg	189.71	J/mol×K	511.07	Joback Method
cpg	194.67	J/mol×K	544.39	Joback Method
cpg	199.37	J/mol×K	577.71	Joback Method
cpg	203.82	J/mol×K	611.03	Joback Method
cpg	208.04	J/mol×K	644.36	Joback Method
cpg	212.01	J/mol×K	677.68	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C827156&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method: https://en.wikipedia.org/wiki/Joback_method

Legend

chl: Standard liquid enthalpy of combustion
cpg: Ideal gas heat capacity
ea: Electron affinity
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
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
tc: Critical Temperature
tf: Normal melting (fusion) point

vc: Critical Volume