2,4-Difluoroiodobenzene

Other names: 1,3-Difluoro-4-iodobenzene
Inchi: InChI=1S/C6H3F2I/c7-4-1-2-6(9)5(8)3-4/h1-3H
InchiKey: YKLDMAPEGQYZRT-UHFFFAOYSA-N
Formula: C6H3F2I
SMILES: Fc1ccc(I)c(F)c1
Mol. weight [g/mol]: 239.99
CAS: 2265-93-2

Physical Properties

Property code	Value	Unit	Source
gf	-238.71	kJ/mol	Joback Method
hf	-268.93	kJ/mol	Joback Method
hfus	15.13	kJ/mol	Joback Method
hvap	40.29	kJ/mol	Joback Method
log10ws	-3.28		Crippen Method
logp	2.569		Crippen Method
mcvol	101.000	ml/mol	McGowan Method
pc	3881.95	kPa	Joback Method
tb	465.00	K	Joback Method
tc	696.31	K	Joback Method
tf	268.08	K	Joback Method
vc	0.388	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	160.77	J/mol×K	465.00	Joback Method
cpg	168.32	J/mol×K	503.55	Joback Method
cpg	175.32	J/mol×K	542.10	Joback Method
cpg	181.81	J/mol×K	580.65	Joback Method
cpg	187.81	J/mol×K	619.20	Joback Method
cpg	193.37	J/mol×K	657.75	Joback Method
cpg	198.50	J/mol×K	696.31	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	348.00	K	3.30	NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C2265932&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

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
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