2-Bromo-4,6-difluoroiodobenzene

Inchi: InChI=1S/C6H2BrF2I/c7-4-1-3(8)2-5(9)6(4)10/h1-2H
InchiKey: KJJGFGWQNCPZBG-UHFFFAOYSA-N
Formula: C6H2BrF2I
SMILES: Fc1cc(F)c(I)c(Br)c1
Mol. weight [g/mol]: 318.88
CAS: 175278-11-2

Physical Properties

Property code	Value	Unit	Source
gf	-234.02	kJ/mol	Joback Method
hf	-254.07	kJ/mol	Joback Method
hfus	20.02	kJ/mol	Joback Method
hvap	47.39	kJ/mol	Joback Method
log10ws	-4.45		Crippen Method
logp	3.332		Crippen Method
mcvol	118.500	ml/mol	McGowan Method
pc	4156.97	kPa	Joback Method
tb	536.14	K	Joback Method
tc	785.66	K	Joback Method
tf	340.40	K	Joback Method
vc	0.450	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	185.50	J/mol×K	536.14	Joback Method
cpg	191.84	J/mol×K	577.73	Joback Method
cpg	197.64	J/mol×K	619.31	Joback Method
cpg	202.97	J/mol×K	660.90	Joback Method
cpg	207.85	J/mol×K	702.48	Joback Method
cpg	212.33	J/mol×K	744.07	Joback Method
cpg	216.46	J/mol×K	785.66	Joback Method

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C175278112&Units=SI

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
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume