4-Bromo-2-fluoroaniline

Other names: Benzenamine, 4-bromo-2-fluoro-
Inchi: InChI=1S/C6H5BrFN/c7-4-1-2-6(9)5(8)3-4/h1-3H,9H2
InchiKey: GZRMNMGWNKSANY-UHFFFAOYSA-N
Formula: C6H5BrFN
SMILES: Nc1ccc(Br)cc1F
Mol. weight [g/mol]: 190.01
CAS: 367-24-8

Physical Properties

Property code	Value	Unit	Source
gf	-21.25	kJ/mol	Joback Method
hf	-89.57	kJ/mol	Joback Method
hfus	18.12	kJ/mol	Joback Method
hvap	48.81	kJ/mol	Joback Method
log10ws	-2.60		Crippen Method
logp	2.170		Crippen Method
mcvol	100.890	ml/mol	McGowan Method
pc	5015.69	kPa	Joback Method
tb	511.28	K	Joback Method
tc	748.98	K	Joback Method
tf	352.49	K	Joback Method
vc	0.372	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	187.37	J/mol×K	511.28	Joback Method
cpg	195.68	J/mol×K	550.90	Joback Method
cpg	203.39	J/mol×K	590.51	Joback Method
cpg	210.55	J/mol×K	630.13	Joback Method
cpg	217.18	J/mol×K	669.75	Joback Method
cpg	223.32	J/mol×K	709.37	Joback Method
cpg	229.00	J/mol×K	748.98	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=C367248&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

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