2-Bromo-6-chloro-4-fluoroaniline

Other names: Benzenamine, 2-bromo-6-chloro-4-fluoro-
Inchi: InChI=1S/C6H4BrClFN/c7-4-1-3(9)2-5(8)6(4)10/h1-2H,10H2
InchiKey: LIBGMUMMWYKJSC-UHFFFAOYSA-N
Formula: C6H4BrClFN
SMILES: Nc1c(Cl)cc(F)cc1Br
Mol. weight [g/mol]: 224.46
CAS: 201849-14-1

Physical Properties

Property code	Value	Unit	Source
gf	-42.81	kJ/mol	Joback Method
hf	-116.78	kJ/mol	Joback Method
hfus	21.93	kJ/mol	Joback Method
hvap	53.86	kJ/mol	Joback Method
log10ws	-3.28		Crippen Method
logp	2.824		Crippen Method
mcvol	113.130	ml/mol	McGowan Method
pc	4665.71	kPa	Joback Method
tb	553.69	K	Joback Method
tc	797.23	K	Joback Method
tf	394.93	K	Joback Method
vc	0.421	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	205.85	J/mol×K	553.69	Joback Method
cpg	213.10	J/mol×K	594.28	Joback Method
cpg	219.83	J/mol×K	634.87	Joback Method
cpg	226.07	J/mol×K	675.46	Joback Method
cpg	231.84	J/mol×K	716.05	Joback Method
cpg	237.18	J/mol×K	756.64	Joback Method
cpg	242.11	J/mol×K	797.23	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C201849141&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
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume