5-Bromo-2-fluorobenzonitrile

Other names: Benzonitrile, 5-bromo-2-fluoro-
Inchi: InChI=1S/C7H3BrFN/c8-6-1-2-7(9)5(3-6)4-10/h1-3H
InchiKey: GYCNHFWRPJXTSB-UHFFFAOYSA-N
Formula: C7H3BrFN
SMILES: N#Cc1cc(Br)ccc1F
Mol. weight [g/mol]: 200.01
CAS: 179897-89-3

Physical Properties

Property code	Value	Unit	Source
gf	53.90	kJ/mol	Joback Method
hf	20.88	kJ/mol	Joback Method
hfus	17.02	kJ/mol	Joback Method
hvap	50.87	kJ/mol	Joback Method
log10ws	-3.32		Crippen Method
logp	2.460		Crippen Method
mcvol	106.380	ml/mol	McGowan Method
pc	3955.54	kPa	Joback Method
tb	563.71	K	Joback Method
tc	804.70	K	Joback Method
tf	345.49	K	Joback Method
vc	0.425	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	195.13	J/mol×K	563.71	Joback Method
cpg	202.19	J/mol×K	603.87	Joback Method
cpg	208.71	J/mol×K	644.04	Joback Method
cpg	214.75	J/mol×K	684.20	Joback Method
cpg	220.31	J/mol×K	724.37	Joback Method
cpg	225.45	J/mol×K	764.53	Joback Method
cpg	230.18	J/mol×K	804.70	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C179897893&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