

3-bromo-4-fluorobenzonitrile

Inchi:	InChI=1S/C7H3BrFN/c8-6-3-5(4-10)1-2-7(6)9/h1-3H
InchiKey:	JKCYKISVUIVZCS-UHFFFAOYSA-N
Formula:	C7H3BrFN
SMILES:	N#Cc1ccc(F)c(Br)c1
Mol. weight [g/mol]:	200.01
CAS:	79630-23-2

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	m ³ /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

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C79630232&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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

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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