4-Bromo-2-methylbenzonitrile

Inchi: InChI=1S/C8H6BrN/c1-6-4-8(9)3-2-7(6)5-10/h2-4H,1H3
InchiKey: LPEBMDFRIKYFCF-UHFFFAOYSA-N
Formula: C8H6BrN
SMILES: Cc1cc(Br)ccc1C#N
Mol. weight [g/mol]: 196.04
CAS: 67832-11-5

Physical Properties

Property code	Value	Unit	Source
gf	257.13	kJ/mol	Joback Method
hf	196.35	kJ/mol	Joback Method
hfus	16.53	kJ/mol	Joback Method
hvap	53.92	kJ/mol	Joback Method
log10ws	-3.46		Crippen Method
logp	2.629		Crippen Method
mcvol	118.700	ml/mol	McGowan Method
pc	3713.49	kPa	Joback Method
tb	587.32	K	Joback Method
tc	835.97	K	Joback Method
tf	356.17	K	Joback Method
vc	0.464	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	229.39	J/mol×K	587.32	Joback Method
cpg	238.16	J/mol×K	628.76	Joback Method
cpg	246.30	J/mol×K	670.20	Joback Method
cpg	253.85	J/mol×K	711.64	Joback Method
cpg	260.84	J/mol×K	753.09	Joback Method
cpg	267.31	J/mol×K	794.53	Joback Method
cpg	273.30	J/mol×K	835.97	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=C67832115&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