4-Bromo-2-ethylaniline

Other names: Benzenamine, 4-bromo-2-ethyl-
Inchi: InChI=1S/C8H10BrN/c1-2-6-5-7(9)3-4-8(6)10/h3-5H,2,10H2,1H3
InchiKey: LGOZNQPHTIGMQJ-UHFFFAOYSA-N
Formula: C8H10BrN
SMILES: CCc1cc(Br)ccc1N
Mol. weight [g/mol]: 200.08
CAS: 45762-41-2

Physical Properties

Property code	Value	Unit	Source
gf	190.40	kJ/mol	Joback Method
hf	65.26	kJ/mol	Joback Method
hfus	20.22	kJ/mol	Joback Method
hvap	54.08	kJ/mol	Joback Method
log10ws	-3.07		Crippen Method
logp	2.594		Crippen Method
mcvol	127.300	ml/mol	McGowan Method
pc	4114.41	kPa	Joback Method
tb	557.77	K	Joback Method
tc	798.87	K	Joback Method
tf	374.44	K	Joback Method
vc	0.467	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	262.96	J/mol×K	557.77	Joback Method
cpg	274.29	J/mol×K	597.95	Joback Method
cpg	284.85	J/mol×K	638.14	Joback Method
cpg	294.70	J/mol×K	678.32	Joback Method
cpg	303.86	J/mol×K	718.51	Joback Method
cpg	312.39	J/mol×K	758.69	Joback Method
cpg	320.33	J/mol×K	798.87	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=C45762412&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