4-Bromo-N,N-diethylaniline

Other names:	p-Bromo-N,N-diethylaniline
	Benzenamine, 4-bromo-N,N-diethyl-
	Aniline, p-bromo-N,N-diethyl-
	p-N,Nddiethylaniline
Inchi:	InChI=1S/C10H14BrN/c1-3-12(4-2)10-7-5-9(11)6-8-10/h5-8H,3-4H2,1-2H3
InchiKey:	NGYMZFJVHHKJQR-UHFFFAOYSA-N
Formula:	C10H14BrN
SMILES:	CCN(CC)c1ccc(Br)cc1
Mol. weight [g/mol]:	228.13
CAS:	2052-06-4

Physical Properties

Property code	Value	Unit	Source
gf	261.20	kJ/mol	Joback Method
hf	69.19	kJ/mol	Joback Method
hfus	23.61	kJ/mol	Joback Method
hvap	49.27	kJ/mol	Joback Method
ie	6.96	eV	NIST Webbook
log10ws	-3.38		Crippen Method
logp	3.295		Crippen Method
mcvol	155.480	ml/mol	McGowan Method
pc	3103.64	kPa	Joback Method
tb	543.20	K	NIST Webbook
tc	757.07	K	Joback Method
tf	333.67	K	Joback Method
vc	0.568	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	332.36	J/mol×K	538.46	Joback Method
cpg	346.96	J/mol×K	574.89	Joback Method
cpg	360.61	J/mol×K	611.33	Joback Method
cpg	373.36	J/mol×K	647.76	Joback Method

cpg	385.27	J/mol×K	684.20	Joback Method
cpg	396.38	J/mol×K	720.63	Joback Method
cpg	406.75	J/mol×K	757.07	Joback Method

Sources

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=C2052064&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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
ie:	Ionization energy
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