

3,4-Dibromoaniline

Other names:	Benzenamine, 3,4-dibromo-
Inchi:	InChI=1S/C6H5Br2N/c7-5-2-1-4(9)3-6(5)8/h1-3H,9H2
InchiKey:	QFTJOYLPELHHCO-UHFFFAOYSA-N
Formula:	C6H5Br2N
SMILES:	Nc1ccc(Br)c(Br)c1
Mol. weight [g/mol]:	250.92
CAS:	615-55-4

Physical Properties

Property code	Value	Unit	Source
gf	187.88	kJ/mol	Joback Method
hf	132.87	kJ/mol	Joback Method
hfus	20.33	kJ/mol	Joback Method
hvap	56.06	kJ/mol	Joback Method
log10ws	-3.43		Crippen Method
logp	2.794		Crippen Method
mcvol	116.620	ml/mol	McGowan Method
pc	5935.41	kPa	Joback Method
tb	578.17	K	Joback Method
tc	844.98	K	Joback Method
tf	411.70	K	Joback Method
vc	0.416	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	205.53	J/molxK	578.17	Joback Method
cpg	213.33	J/molxK	622.64	Joback Method
cpg	220.45	J/molxK	667.11	Joback Method
cpg	226.96	J/molxK	711.58	Joback Method
cpg	232.91	J/molxK	756.05	Joback Method
cpg	238.36	J/molxK	800.52	Joback Method
cpg	243.39	J/molxK	844.98	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=C615554&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
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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