2,6-Dibromo-4-methylaniline

Other names: Benzenamine, 2,6-dibromo-4-methyl-
2,6-Dibromo-p-toludine
2,6-Dibromo-p-toluidine
Inchi: InChI=1S/C7H7Br2N/c1-4-2-5(8)7(10)6(9)3-4/h2-3H,10H2,1H3
InchiKey: ATDIROHVRVQMRO-UHFFFAOYSA-N
Formula: C7H7Br2N
SMILES: Cc1cc(Br)c(N)c(Br)c1
Mol. weight [g/mol]: 264.94
CAS: 6968-24-7

Physical Properties

Property code	Value	Unit	Source
gf	186.67	kJ/mol	Joback Method
hf	100.76	kJ/mol	Joback Method
hfus	22.53	kJ/mol	Joback Method
hvap	58.95	kJ/mol	Joback Method
log10ws	-3.91		Crippen Method
logp	3.102		Crippen Method
mcvol	130.710	ml/mol	McGowan Method
pc	5037.07	kPa	Joback Method
tb	606.03	K	Joback Method
tc	867.57	K	Joback Method
tf	435.49	K	Joback Method
vc	0.472	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	247.17	J/mol×K	606.03	Joback Method
cpg	255.96	J/mol×K	649.62	Joback Method
cpg	264.10	J/mol×K	693.21	Joback Method
cpg	271.62	J/mol×K	736.80	Joback Method
cpg	278.58	J/mol×K	780.39	Joback Method
cpg	285.03	J/mol×K	823.98	Joback Method

cpg	291.02	J/mol×K	867.57	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=C6968247&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