4-Bromo-2,6-dichloroaniline

Other names: Benzenamine, 2-bromo-4,6-dichloro-
2-bromo-4,6-dichloroaniline
Inchi: InChI=1S/C6H4BrCl2N/c7-3-1-4(8)6(10)5(9)2-3/h1-2H,10H2
InchiKey: NPQBZKNXJZARBJ-UHFFFAOYSA-N
Formula: C6H4BrCl2N
SMILES: Nc1c(Cl)cc(Br)cc1Cl
Mol. weight [g/mol]: 240.91
CAS: 697-86-9

Physical Properties

Property code	Value	Unit	Source
gf	140.07	kJ/mol	Joback Method
hf	63.59	kJ/mol	Joback Method
hfus	23.05	kJ/mol	Joback Method
hvap	59.06	kJ/mol	Joback Method
log10ws	-3.64		Crippen Method
logp	3.338		Crippen Method
mcvol	123.600	ml/mol	McGowan Method
pc	4717.12	kPa	Joback Method
tb	591.85	K	Joback Method
tc	852.69	K	Joback Method
tf	424.26	K	Joback Method
vc	0.453	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	215.83	J/mol×K	591.85	Joback Method
cpg	222.78	J/mol×K	635.32	Joback Method
cpg	229.19	J/mol×K	678.80	Joback Method
cpg	235.07	J/mol×K	722.27	Joback Method
cpg	240.47	J/mol×K	765.74	Joback Method
cpg	245.43	J/mol×K	809.22	Joback Method
cpg	249.97	J/mol×K	852.69	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C697869&Units=SI
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

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