4,6-Dibromo-2,3-dichloroaniline

Inchi: InChI=1S/C6H3Br2Cl2N/c7-2-1-3(8)6(11)5(10)4(2)9/h1H,11H2
InchiKey: IPWGDMQXLGFBLC-UHFFFAOYSA-N
Formula: C6H3Br2Cl2N
SMILES: Nc1c(Br)cc(Br)c(Cl)c1Cl
Mol. weight [g/mol]: 319.81
CAS: 113571-15-6

Physical Properties

Property code	Value	Unit	Source
gf	144.76	kJ/mol	Joback Method
hf	78.45	kJ/mol	Joback Method
hfus	27.94	kJ/mol	Joback Method
hvap	66.16	kJ/mol	Joback Method
log10ws	-4.80		Crippen Method
logp	4.101		Crippen Method
mcvol	141.100	ml/mol	McGowan Method
pc	5087.49	kPa	Joback Method
tb	662.99	K	Joback Method
tc	937.34	K	Joback Method
tf	496.58	K	Joback Method
vc	0.514	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	236.05	J/mol×K	662.99	Joback Method
cpg	241.77	J/mol×K	708.71	Joback Method
cpg	247.00	J/mol×K	754.44	Joback Method
cpg	251.80	J/mol×K	800.16	Joback Method
cpg	256.21	J/mol×K	845.89	Joback Method
cpg	260.27	J/mol×K	891.61	Joback Method
cpg	264.05	J/mol×K	937.34	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C113571156&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