3-Chloro-2,6-dibromo-4-methylaniline

Inchi: InChI=1S/C7H6Br2ClN/c1-3-2-4(8)7(11)5(9)6(3)10/h2H,11H2,1H3
InchiKey: XBSGYHXODZBFBM-UHFFFAOYSA-N
Formula: C7H6Br2ClN
SMILES: Cc1cc(Br)c(N)c(Br)c1Cl
Mol. weight [g/mol]: 299.39
CAS: 84483-22-7

Physical Properties

Property code	Value	Unit	Source
gf	165.11	kJ/mol	Joback Method
hf	73.55	kJ/mol	Joback Method
hfus	26.34	kJ/mol	Joback Method
hvap	64.00	kJ/mol	Joback Method
log10ws	-4.59		Crippen Method
logp	3.756		Crippen Method
mcvol	142.950	ml/mol	McGowan Method
pc	4684.89	kPa	Joback Method
tb	648.44	K	Joback Method
tc	913.71	K	Joback Method
tf	477.93	K	Joback Method
vc	0.521	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	264.03	J/mol×K	648.44	Joback Method
cpg	271.78	J/mol×K	692.65	Joback Method
cpg	278.95	J/mol×K	736.86	Joback Method
cpg	285.59	J/mol×K	781.07	Joback Method
cpg	291.74	J/mol×K	825.28	Joback Method
cpg	297.45	J/mol×K	869.50	Joback Method
cpg	302.77	J/mol×K	913.71	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C84483227&Units=SI

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