

4-Bis(2-chloroethyl)aminobenzaldehyde

Other names:	4-(N,N-Bis(2-chloroethyl)amino)benzaldehyde p-N,N-Bis(2-chloroethyl)aminobenzaldehyde p-Bis(«beta»-chloroethyl)aminobenzaldehyde p-Bis(2-chloroethyl)aminobenzaldehyde Benzaldehyde, p-(bis(2-chloroethyl)amino)- Benzaldehyde, 4-(bis(2-chloroethyl)amino)- 4-Aminobenzaldehyde, N,N-di[2-chloroethyl]-
Inchi:	InChI=1S/C11H13Cl2NO/c12-5-7-14(8-6-13)11-3-1-10(9-15)2-4-11/h1-4,9H,5-8H2
InchiKey:	PXUFHXLGUJLBMI-UHFFFAOYSA-N
Formula:	C11H13Cl2NO
SMILES:	O=Cc1ccc(N(CCCI)CCCI)cc1
Mol. weight [g/mol]:	246.13
CAS:	1208-03-3

Physical Properties

Property code	Value	Unit	Source
gf	131.92	kJ/mol	Joback Method
hf	-94.84	kJ/mol	Joback Method
hfus	31.60	kJ/mol	Joback Method
hvap	60.55	kJ/mol	Joback Method
log10ws	-2.76		Crippen Method
logp	2.783		Crippen Method
mcvol	178.120	ml/mol	McGowan Method
pc	2603.08	kPa	Joback Method
tb	618.70	K	Joback Method
tc	831.51	K	Joback Method
tf	386.98	K	Joback Method
vc	0.676	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	411.17	J/mol×K	618.70	Joback Method
cpg	423.99	J/mol×K	654.17	Joback Method

cpg	435.94	J/mol×K	689.64	Joback Method
cpg	447.06	J/mol×K	725.10	Joback Method
cpg	457.42	J/mol×K	760.57	Joback Method
cpg	467.04	J/mol×K	796.04	Joback Method
cpg	475.99	J/mol×K	831.51	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=C1208033&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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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