4-AMINOBENZALDEHYDE, N,N-DI[2-CHLOROETHYL]-

Other names: 4-(N,N-Bis(2-chloroethyl)amino)benzaldehyde
4-Aminobenzaldehyde, N,N-di[2-chloroethyl]-
Benzaldehyde, 4-(bis(2-chloroethyl)amino)-
Benzaldehyde, p-(bis(2-chloroethyl)amino)-
p-Bis(2-chloroethyl)aminobenzaldehyde
p-Bis(«beta»-chloroethyl)aminobenzaldehyde
p-N,N-Bis(2-chloroethyl)aminobenzaldehyde

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(CCCl)CCCl)cc1

Mol. weight [g/mol]: 246.14

Physical Properties

Property code	Value	Unit	Source
hfus	31.60	kJ/mol	Joback Method
ie	8.28	eV	Cheméo Relay (1.0)
logp	2.783		Crippen Method
mcvol	178.120	ml/mol	McGowan Method
tb	604.54	K	Cheméo Relay (1.0)
tf	339.17	K	Cheméo Relay (1.0)

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

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1208033&Units=SI
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
hfus:	Enthalpy of fusion at standard conditions
ie:	Ionization energy
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point