4-N,N-Bis(2-chloroethyl)amino-2-tolualdehyde

Other names: o-Tolualdehyde, 4-(bis(2-chloroethyl)amino)-
Benzaldehyde, 4-[bis(2-chloroethyl)amino]-2-methyl-
Inchi: InChI=1S/C12H15Cl2NO/c1-10-8-12(3-2-11(10)9-16)15(6-4-13)7-5-14/h2-3,8-9H,4-7H2,
InchiKey: ZQIAXDULHBLZJE-UHFFFAOYSA-N
Formula: C12H15Cl2NO
SMILES: Cc1cc(N(CCCl)CCCl)ccc1C=O
Mol. weight [g/mol]: 260.16
CAS: 26459-95-0

Physical Properties

Property code	Value	Unit	Source
gf	130.71	kJ/mol	Joback Method
hf	-126.95	kJ/mol	Joback Method
hfus	33.80	kJ/mol	Joback Method
hvap	63.44	kJ/mol	Joback Method
log10ws	-3.24		Crippen Method
logp	3.092		Crippen Method
mcvol	192.210	ml/mol	McGowan Method
pc	2331.52	kPa	Joback Method
tb	646.56	K	Joback Method
tc	856.87	K	Joback Method
tf	410.77	K	Joback Method
vc	0.733	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	459.44	J/mol×K	646.56	Joback Method
cpg	472.66	J/mol×K	681.61	Joback Method
cpg	485.04	J/mol×K	716.66	Joback Method
cpg	496.61	J/mol×K	751.72	Joback Method
cpg	507.42	J/mol×K	786.77	Joback Method
cpg	517.51	J/mol×K	821.82	Joback Method
cpg	526.92	J/mol×K	856.87	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=C26459950&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