p-([2-Chloroethyl]ethylamino)benzaldehyde

Other names: p-(N-(2-Chloroethyl)-N-ethyl)aminobenzaldehyde
Benzaldehyde, 4-[(2-chloroethyl)ethylamino]-
Inchi: InChI=1S/C11H14ClNO/c1-2-13(8-7-12)11-5-3-10(9-14)4-6-11/h3-6,9H,2,7-8H2,1H3
InchiKey: MFUFJCIFNHFEDW-UHFFFAOYSA-N
Formula: C11H14ClNO
SMILES: CCN(CCCl)c1ccc(C=O)cc1
Mol. weight [g/mol]: 211.69
CAS: 2643-07-4

Physical Properties

Property code	Value	Unit	Source
gf	143.85	kJ/mol	Joback Method
hf	-79.10	kJ/mol	Joback Method
hfus	27.41	kJ/mol	Joback Method
hvap	56.17	kJ/mol	Joback Method
log10ws	-2.61		Crippen Method
logp	2.564		Crippen Method
mcvol	165.880	ml/mol	McGowan Method
pc	2704.22	kPa	Joback Method
tb	581.27	K	Joback Method
tc	790.22	K	Joback Method
tf	357.06	K	Joback Method
vc	0.627	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	384.95	J/mol×K	581.27	Joback Method
cpg	398.77	J/mol×K	616.09	Joback Method
cpg	411.71	J/mol×K	650.92	Joback Method
cpg	423.82	J/mol×K	685.74	Joback Method
cpg	435.13	J/mol×K	720.57	Joback Method
cpg	445.70	J/mol×K	755.39	Joback Method
cpg	455.56	J/mol×K	790.22	Joback Method

Sources

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=C2643074&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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