N-(beta-diethylaminoethyl)-2-chloro-4-aminobenza

Inchi: InChI=1S/C13H20ClN3O/c1-3-17(4-2)8-7-16-13(18)11-6-5-10(15)9-12(11)14/h5-6,9H,3-4

InchiKey: JXLOEMYUSALHDJ-UHFFFAOYSA-N

Formula: C13H20ClN3O

SMILES: CCN(CC)CCNC(=O)c1ccc(N)cc1Cl

Mol. weight [g/mol]: 269.77

CAS: 840-10-8

Physical Properties

Property code	Value	Unit	Source
gf	277.50	kJ/mol	Joback Method
hf	-71.59	kJ/mol	Joback Method
hfus	41.80	kJ/mol	Joback Method
hvap	78.38	kJ/mol	Joback Method
log10ws	-2.80		Crippen Method
logp	1.994		Crippen Method
mcvol	214.020	ml/mol	McGowan Method
pc	2331.52	kPa	Joback Method
tb	759.92	K	Joback Method
tc	974.33	K	Joback Method
tf	535.97	K	Joback Method
vc	0.792	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	598.39	J/mol×K	759.92	Joback Method
cpg	612.01	J/mol×K	795.65	Joback Method
cpg	624.70	J/mol×K	831.39	Joback Method
cpg	636.51	J/mol×K	867.12	Joback Method
cpg	647.50	J/mol×K	902.86	Joback Method
cpg	657.71	J/mol×K	938.59	Joback Method
cpg	667.19	J/mol×K	974.33	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=C840108&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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