2-Chloro-N,N-dimethyl-4-nitroaniline

Other names: Benzenamine, 2-chloro-N,N-dimethyl-4-nitro-
Inchi: InChI=1S/C8H9ClN2O2/c1-10(2)8-4-3-6(11(12)13)5-7(8)9/h3-5H,1-2H3
InchiKey: OZKAWTHGBGLZKC-UHFFFAOYSA-N
Formula: C8H9ClN2O2
SMILES: CN(C)c1ccc([N+](=O)[O-])cc1Cl
Mol. weight [g/mol]: 200.62
CAS: 6213-19-0

Physical Properties

Property code	Value	Unit	Source
gf	244.03	kJ/mol	Joback Method
hf	46.17	kJ/mol	Joback Method
hfus	28.32	kJ/mol	Joback Method
hvap	60.02	kJ/mol	Joback Method
log10ws	-2.72		Crippen Method
logp	2.314		Crippen Method
mcvol	139.460	ml/mol	McGowan Method
pc	3411.87	kPa	Joback Method
tb	620.79	K	Joback Method
tc	865.65	K	Joback Method
tf	437.38	K	Joback Method
vc	0.524	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	321.90	J/mol×K	620.79	Joback Method
cpg	333.52	J/mol×K	661.60	Joback Method
cpg	344.23	J/mol×K	702.41	Joback Method
cpg	354.10	J/mol×K	743.22	Joback Method
cpg	363.17	J/mol×K	784.03	Joback Method
cpg	371.49	J/mol×K	824.84	Joback Method
cpg	379.12	J/mol×K	865.65	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=C6213190&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