Benzenamine, 4-chloro-3-nitro-

Other names: Aniline, 4-chloro-3-nitro-
4-Chloro-3-nitroaniline
Inchi: InChI=1S/C6H5ClN2O2/c7-5-2-1-4(8)3-6(5)9(10)11/h1-3H,8H2
InchiKey: FOHHWGVAOVDVLP-UHFFFAOYSA-N
Formula: C6H5ClN2O2
SMILES: Nc1ccc(Cl)c([N+](=O)[O-])c1
Mol. weight [g/mol]: 172.57
CAS: 635-22-3

Physical Properties

Property code	Value	Unit	Source
gf	182.86	kJ/mol	Joback Method
hf	53.71	kJ/mol	Joback Method
hfus	25.31	kJ/mol	Joback Method
hvap	64.17	kJ/mol	Joback Method
log10ws	-2.44		Crippen Method
logp	1.830		Crippen Method
mcvol	111.280	ml/mol	McGowan Method
pc	4684.89	kPa	Joback Method
tb	635.12	K	Joback Method
tc	902.71	K	Joback Method
tf	465.63	K	Joback Method
vc	0.423	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	243.95	J/mol×K	635.12	Joback Method
cpg	252.54	J/mol×K	679.72	Joback Method
cpg	260.38	J/mol×K	724.32	Joback Method
cpg	267.52	J/mol×K	768.91	Joback Method
cpg	273.99	J/mol×K	813.51	Joback Method
cpg	279.84	J/mol×K	858.11	Joback Method
cpg	285.10	J/mol×K	902.71	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=C635223&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