Benzenamine, 4-chloro-2-nitro-N-phenyl-

Other names: N-(4-Chloro-2-nitrophenyl)aniline
4-Chloro-2-nitrodiphenylamine
4-chloro-2-nitro-N-phenylaniline
Inchi: InChI=1S/C12H9ClN2O2/c13-9-6-7-11(12(8-9)15(16)17)14-10-4-2-1-3-5-10/h1-8,14H
InchiKey: GYOVQZDXSHTPBS-UHFFFAOYSA-N
Formula: C12H9ClN2O2
SMILES: O=[N+]([O-])c1cc(Cl)ccc1Nc1ccccc1
Mol. weight [g/mol]: 248.66
CAS: 16611-15-7

Physical Properties

Property code	Value	Unit	Source
gf	368.73	kJ/mol	Joback Method
hf	186.08	kJ/mol	Joback Method
hfus	34.80	kJ/mol	Joback Method
hvap	75.59	kJ/mol	Joback Method
log10ws	-4.61		Crippen Method
logp	3.992		Crippen Method
mcvol	172.060	ml/mol	McGowan Method
pc	3265.31	kPa	Joback Method
tb	776.72	K	Joback Method
tc	1048.73	K	Joback Method
tf	529.07	K	Joback Method
vc	0.657	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	440.49	J/mol×K	776.72	Joback Method
cpg	451.95	J/mol×K	822.05	Joback Method
cpg	462.25	J/mol×K	867.39	Joback Method
cpg	471.50	J/mol×K	912.72	Joback Method
cpg	479.78	J/mol×K	958.06	Joback Method
cpg	487.21	J/mol×K	1003.39	Joback Method

cpg	493.86	J/mol×K	1048.73	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C16611157&Units=SI
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

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