5-Chloro-3-nitro-o-phenylene diamine

Inchi: InChI=1S/C6H6ClN3O2/c7-3-1-4(8)6(9)5(2-3)10(11)12/h1-2H,8-9H2
InchiKey: PIPKLZRJGNJMBY-UHFFFAOYSA-N
Formula: C6H6ClN3O2
SMILES: Nc1cc(Cl)cc([N+](=O)[O-])c1N
Mol. weight [g/mol]: 187.58
CAS: 42389-30-0

Physical Properties

Property code	Value	Unit	Source
gf	239.68	kJ/mol	Joback Method
hf	76.03	kJ/mol	Joback Method
hfus	30.12	kJ/mol	Joback Method
hvap	75.47	kJ/mol	Joback Method
log10ws	-2.08		Crippen Method
logp	1.413		Crippen Method
mcvol	121.260	ml/mol	McGowan Method
pc	4966.33	kPa	Joback Method
tb	712.63	K	Joback Method
tc	985.51	K	Joback Method
tf	561.41	K	Joback Method
vc	0.453	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	287.87	J/mol×K	712.63	Joback Method
cpg	295.99	J/mol×K	758.11	Joback Method
cpg	303.38	J/mol×K	803.59	Joback Method
cpg	310.06	J/mol×K	849.07	Joback Method
cpg	316.08	J/mol×K	894.55	Joback Method
cpg	321.47	J/mol×K	940.03	Joback Method
cpg	326.26	J/mol×K	985.51	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C42389300&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