Benzenamine, 2-chloro-5-nitro-

Other names:	2-Chloro-5-nitroaniline
	3-Nitro-6-chloroaniline
	6-Chloro-3-nitroaniline
	Aniline, 2-chloro-5-nitro-
Inchi:	InChI=1S/C6H5ClN2O2/c7-5-2-1-4(9(10)11)3-6(5)8/h1-3H,8H2
InchiKey:	KWIXNFOTNVKIGM-UHFFFAOYSA-N
Formula:	C6H5ClN2O2
SMILES:	Nc1cc([N+](=O)[O-])ccc1Cl
Mol. weight [g/mol]:	172.57
CAS:	6283-25-6

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
hsub	101.00 ± 1.60	kJ/mol	NIST Webbook
hsub	100.30 ± 2.20	kJ/mol	NIST Webbook
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
tt	393.39	K	Solubility Measurement and Thermodynamic Model Correlation and Evaluation of 2-Chloro-5-nitroaniline in 12 Pure Solvents
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
hsubt	99.30 ± 1.60	kJ/mol	333.00	NIST Webbook

Sources

Solubility Measurement and Thermodynamic Model Correlation and Evaluation of 2-Chloro-5-nitroaniline in 12 Pure Solvents:	https://www.doi.org/10.1021/acs.jced.8b00931
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=C6283256&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
hsub:	Enthalpy of sublimation at standard conditions
hsubt:	Enthalpy of sublimation at a given temperature
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
tt:	Triple Point Temperature
vc:	Critical Volume