1-Chloro-2,6-dinitrobenzene

Other names: Benzene, 2-chloro-1,3-dinitro-
1,3-Dinitro-2-chlorobenzene
2-Chloro-1,3-dinitrobenzene
2-Chloro-1,3-dintrobenzene
2,6-Dinitrochlorobenzene
Inchi: InChI=1S/C6H3ClN2O4/c7-6-4(8(10)11)2-1-3-5(6)9(12)13/h1-3H
InchiKey: BPPMIQPXQVIZNJ-UHFFFAOYSA-N
Formula: C6H3ClN2O4
SMILES: O=[N+]([O-])c1cccc([N+](=O)[O-])c1Cl
Mol. weight [g/mol]: 202.55
CAS: 606-21-3

Physical Properties

Property code	Value	Unit	Source
gf	151.96	kJ/mol	Joback Method
hf	9.16	kJ/mol	Joback Method
hfus	31.48	kJ/mol	Joback Method
hvap	70.12	kJ/mol	Joback Method
log10ws	-3.46		Crippen Method
logp	2.156		Crippen Method
mcvol	118.720	ml/mol	McGowan Method
pc	4409.10	kPa	Joback Method
tb	714.43	K	Joback Method
tc	997.45	K	Joback Method
tf	525.98	K	Joback Method
vc	0.476	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	269.81	J/mol×K	714.43	Joback Method
cpg	277.51	J/mol×K	761.60	Joback Method
cpg	284.39	J/mol×K	808.77	Joback Method
cpg	290.51	J/mol×K	855.94	Joback Method

cpg	295.91	J/mol×K	903.11	Joback Method
cpg	300.65	J/mol×K	950.28	Joback Method
cpg	304.79	J/mol×K	997.45	Joback Method
hfust	18.95	kJ/mol	361.20	NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C606213&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
hfust:	Enthalpy of fusion 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
vc:	Critical Volume