1,3-Dichloro-4,6-dinitrobenzene

Other names:	1,5-Dichloro-2,4-dinitrobenzene
	Benzene, 1,5-dichloro-2,4-dinitro-
	2,4-Dichloro-1,5-dinitrobenzene
	4,6-Dichloro-1,3-dinitrobenzene
	Benzene, 1,3-dichloro-4,6-dinitro-
Inchi:	InChI=1S/C6H2Cl2N2O4/c7-3-1-4(8)6(10(13)14)2-5(3)9(11)12/h1-2H
InchiKey:	ZPXDNSYFDIHPOJ-UHFFFAOYSA-N
Formula:	C6H2Cl2N2O4
SMILES:	O=[N+]([O-])c1cc([N+](=O)[O-])c(Cl)cc1Cl
Mol. weight [g/mol]:	237.00
CAS:	3698-83-7

Physical Properties

Property code	Value	Unit	Source
gf	130.40	kJ/mol	Joback Method
hf	-18.05	kJ/mol	Joback Method
hfus	35.29	kJ/mol	Joback Method
hvap	75.16	kJ/mol	Joback Method
log10ws	-4.14		Crippen Method
logp	2.810		Crippen Method
mcvol	130.960	ml/mol	McGowan Method
pc	4119.70	kPa	Joback Method
tb	756.84	K	Joback Method
tc	1041.75	K	Joback Method
tf	568.42	K	Joback Method
vc	0.525	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	283.90	J/mol×K	756.84	Joback Method
cpg	290.48	J/mol×K	804.33	Joback Method
cpg	296.31	J/mol×K	851.81	Joback Method
cpg	301.45	J/mol×K	899.30	Joback Method

cpg	305.93	J/mol×K	946.78	Joback Method
cpg	309.80	J/mol×K	994.27	Joback Method
cpg	313.11	J/mol×K	1041.75	Joback Method

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
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=C3698837&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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