4-chloro-2,6-dinitroaniline

Inchi: InChI=1S/C6H4ClN3O4/c7-3-1-4(9(11)12)6(8)5(2-3)10(13)14/h1-2H,8H2
InchiKey: CLMQUEQFVUMDPC-UHFFFAOYSA-N
Formula: C6H4ClN3O4
SMILES: Nc1c([N+](=O)[O-])cc(Cl)cc1[N+](=O)[O-]
Mol. weight [g/mol]: 217.57
CAS: 5388-62-5

Physical Properties

Property code	Value	Unit	Source
gf	208.78	kJ/mol	Joback Method
hf	31.48	kJ/mol	Joback Method
hfus	36.29	kJ/mol	Joback Method
hsub	105.20 ± 0.70	kJ/mol	NIST Webbook
hvap	81.42	kJ/mol	Joback Method
log10ws	-3.09		Crippen Method
logp	1.739		Crippen Method
mcvol	128.700	ml/mol	McGowan Method
pc	4665.71	kPa	Joback Method
tb	791.94	K	Joback Method
tc	1078.04	K	Joback Method
tf	621.76	K	Joback Method
vc	0.505	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	340.51	J/mol×K	1030.36	Joback Method
cpg	312.64	J/mol×K	791.94	Joback Method
cpg	319.72	J/mol×K	839.62	Joback Method
cpg	326.00	J/mol×K	887.31	Joback Method
cpg	331.52	J/mol×K	934.99	Joback Method
cpg	336.34	J/mol×K	982.67	Joback Method
cpg	344.05	J/mol×K	1078.04	Joback Method
hsubt	104.70 ± 0.40	kJ/mol	347.00	NIST Webbook

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C5388625&Units=SI&Mask=3FFF

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
vc:	Critical Volume