4,5-Dichloro-2-nitroaniline

Other names: Benzenamine, 4,5-dichloro-2-nitro-
Inchi: InChI=1S/C6H4Cl2N2O2/c7-3-1-5(9)6(10(11)12)2-4(3)8/h1-2H,9H2
InchiKey: FSGTULQLEVAYRS-UHFFFAOYSA-N
Formula: C6H4Cl2N2O2
SMILES: Nc1cc(Cl)c(Cl)cc1[N+](=O)[O-]
Mol. weight [g/mol]: 207.01
CAS: 6641-64-1

Physical Properties

Property code	Value	Unit	Source
gf	161.30	kJ/mol	Joback Method
hf	26.50	kJ/mol	Joback Method
hfus	29.12	kJ/mol	Joback Method
hsub	109.40 ± 0.90	kJ/mol	NIST Webbook
hvap	69.21	kJ/mol	Joback Method
log10ws	-3.13		Crippen Method
logp	2.484		Crippen Method
mcvol	123.520	ml/mol	McGowan Method
pc	4368.40	kPa	Joback Method
tb	677.53	K	Joback Method
tc	948.30	K	Joback Method
tf	508.07	K	Joback Method
vc	0.472	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	260.08	J/mol×K	677.53	Joback Method
cpg	267.57	J/mol×K	722.66	Joback Method
cpg	274.37	J/mol×K	767.79	Joback Method
cpg	280.54	J/mol×K	812.91	Joback Method
cpg	286.09	J/mol×K	858.04	Joback Method
cpg	291.07	J/mol×K	903.17	Joback Method
cpg	295.51	J/mol×K	948.30	Joback Method

hsubt	108.40 ± 0.70	kJ/mol	359.00	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=C6641641&Units=SI

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