Benzene, 1,2-dichloro-4-nitro-

Other names:	1,2-DICHLORO-4-NITROBENZENE
	1-NITRO-3,4-DICHLOROBENZENE
	3,4-dichloronitrobenzene
	DCNB
Inchi:	InChI=1S/C6H3Cl2NO2/c7-5-2-1-4(9(10)11)3-6(5)8/h1-3H
InchiKey:	NTBYINQTYWZXLH-UHFFFAOYSA-N
Formula:	C6H3Cl2NO2
SMILES:	O=[N+]([O-])c1ccc(Cl)c(Cl)c1
Mol. weight [g/mol]:	192.00
CAS:	99-54-7

Physical Properties

Property code	Value	Unit	Source
chs	-2727.40 ± 3.40	kJ/mol	NIST Webbook
ea	1.44 ± 0.05	eV	NIST Webbook
gf	104.48	kJ/mol	Joback Method
hf	4.18	kJ/mol	Joback Method
hfs	-109.70	kJ/mol	NIST Webbook
hfus	24.31	kJ/mol	Joback Method
hsub	85.80 ± 2.50	kJ/mol	NIST Webbook
hsub	83.10 ± 0.60	kJ/mol	NIST Webbook
hvap	65.20 ± 0.20	kJ/mol	NIST Webbook
log10ws	-3.20		Aqueous Solubility Prediction Method
log10ws	-3.20		Estimated Solubility Method
logp	2.902		Crippen Method
mcvol	113.540	ml/mol	McGowan Method
pc	4135.61	kPa	Joback Method
tb	528.70	K	NIST Webbook
tc	864.46	K	Joback Method
tf	314.19	K	Aqueous Solubility Prediction Method
vc	0.444	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	250.50	J/mol×K	820.39	Joback Method
cpg	217.83	J/mol×K	600.02	Joback Method
cpg	225.66	J/mol×K	644.09	Joback Method
cpg	232.80	J/mol×K	688.17	Joback Method
cpg	239.30	J/mol×K	732.24	Joback Method
cpg	245.19	J/mol×K	776.31	Joback Method
cpg	255.28	J/mol×K	864.46	Joback Method
hfust	17.95	kJ/mol	314.10	NIST Webbook
hfust	17.60	kJ/mol	316.00	NIST Webbook
hvapt	55.50	kJ/mol	466.00	NIST Webbook

Sources

Joback Method: https://en.wikipedia.org/wiki/Joback_method
KDB: https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1794
Aqueous Solubility Prediction Method: http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
Estimated Solubility Method: http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C99547&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

chs: Standard solid enthalpy of combustion
cpg: Ideal gas heat capacity
ea: Electron affinity
gf: Standard Gibbs free energy of formation
hf: Enthalpy of formation at standard conditions
hfs: Solid phase enthalpy of formation at standard conditions
hfus: Enthalpy of fusion at standard conditions
hfust: Enthalpy of fusion at a given temperature
hsub: Enthalpy of sublimation at standard conditions
hvap: Enthalpy of vaporization at standard conditions

hvapt:	Enthalpy of vaporization at a given temperature
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