Benzene, 1,2-dichloro-3-nitro-

Other names: 1,2-Dichloro-3-nitrobenzene
2,3-Dichloro-1-nitrobenzene
2,3-Dichloronitrobenzene
Inchi: InChI=1S/C6H3Cl2NO2/c7-4-2-1-3-5(6(4)8)9(10)11/h1-3H
InchiKey: CMVQZRLQEOAYSW-UHFFFAOYSA-N
Formula: C6H3Cl2NO2
SMILES: O=[N+]([O-])c1cccc(Cl)c1Cl
Mol. weight [g/mol]: 192.00
CAS: 3209-22-1

Physical Properties

Property code	Value	Unit	Source
ea	1.29 ± 0.05	eV	NIST Webbook
gf	104.48	kJ/mol	Joback Method
hf	4.18	kJ/mol	Joback Method
hfus	24.31	kJ/mol	Joback Method
hvap	57.91	kJ/mol	Joback Method
log10ws	-3.48		Aqueous Solubility Prediction Method
log10ws	-3.48		Estimated Solubility Method
logp	2.902		Crippen Method
mcvol	113.540	ml/mol	McGowan Method
pc	4135.61	kPa	Joback Method
rinpol	241.00		NIST Webbook
rinpol	1344.00		NIST Webbook
rinpol	241.00		NIST Webbook
rinpol	1344.00		NIST Webbook
ripol	2137.00		NIST Webbook
ripol	2137.00		NIST Webbook
tb	530.70	K	NIST Webbook
tc	864.46	K	Joback Method
tf	333.52 ± 0.25	K	NIST Webbook
tf	334.05 ± 0.15	K	NIST Webbook
tf	333.00 ± 2.00	K	NIST Webbook
tf	334.98	K	Aqueous Solubility Prediction Method

tf	334.90	K	Solubility of Dichloronitrobenzene in Eight Organic Solvents from T = (278.15 to 303.15) K: Measurement and Thermodynamic Modeling
vc	0.444	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
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	250.50	J/mol×K	820.39	Joback Method
cpg	255.28	J/mol×K	864.46	Joback Method
rhol	1533.00	kg/m3	348.15	Vapor pressure and isobaric vapor-liquid equilibrium for dichloronitrobenzene isomers

Sources

Estimated Solubility Method:	http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt
Vapor pressure and isobaric vapor-liquid equilibrium for dichloronitrobenzene isomers:	https://www.doi.org/10.1016/j.fluid.2014.01.034
Experimental Measurement and Modeling of Solubility Data for 2,5-Dichloronitrobenzene in Methanol, Ethanol, and Liquid Mixtures (Methanol + Water, Ethanol + Water):	https://www.doi.org/10.1021/je500494d
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C3209221&Units=SI
Solubility of Dichloronitrobenzene in Eight Organic Solvents from T = (278.15 to 303.15) K: Measurement and Thermodynamic Modeling:	https://www.doi.org/10.1021/je401044h
Measurement and calculation of solid-liquid equilibrium for ternary systems of 3,4-dichloronitrobenzene + 2,3-dichloronitrobenzene + ethanol/n-propanol:	https://www.doi.org/10.1016/j.jct.2016.03.024

Legend

cpg:	Ideal gas heat capacity
ea:	Electron affinity
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
rhol:	Liquid Density
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume