

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

Other names:	Nitro-p-dichlorobenzene 1,4-Dichloro-2-nitrobenzene 2,5-Dichloronitrobenzene Benzene, 2,5-dichloronitro- 1-Nitro-2,5-dichlorobenzene 2,5-Dichlornitrobenzen Benzene, 1-nitro-2,5-dichloro- NSC 406125 2,5-dichloronitrobenzene
Inchi:	InChI=1S/C6H3Cl2NO2/c7-4-1-2-5(8)6(3-4)9(10)11/h1-3H
InchiKey:	RZKKOBGFC AHL CZ-UHFFFAOYSA-N
Formula:	C6H3Cl2NO2
SMILES:	O=[N+](O-)[c1cc(Cl)ccc1Cl]
Mol. weight [g/mol]:	192.00
CAS:	89-61-2

Physical Properties

Property code	Value	Unit	Source
gf	104.48	kJ/mol	Joback Method
hf	4.18	kJ/mol	Joback Method
hfus	24.31	kJ/mol	Joback Method
hsub	87.40 ± 2.40	kJ/mol	NIST Webbook
hvap	57.91	kJ/mol	Joback Method
log10ws	-3.49		Crippen Method
logp	2.902		Crippen Method
mcvol	113.540	ml/mol	McGowan Method
pc	4135.61	kPa	Joback Method
tb	540.20	K	NIST Webbook
tc	864.46	K	Joback Method
tf	326.65 ± 0.20	K	NIST Webbook
tf	326.75 ± 0.15	K	NIST Webbook
tf	327.00 ± 2.00	K	NIST Webbook
vc	0.444	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	217.83	J/molxK	600.02	Joback Method
cpg	225.66	J/molxK	644.09	Joback Method
cpg	232.80	J/molxK	688.17	Joback Method
cpg	239.30	J/molxK	732.24	Joback Method
cpg	245.19	J/molxK	776.31	Joback Method
cpg	250.50	J/molxK	820.39	Joback Method
cpg	255.28	J/molxK	864.46	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=C89612&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
hsub:	Enthalpy of sublimation 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

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