Benzene, 1-chloro-2,4-dinitro-

Other names:	1,3-DINITRO-4-CHLOROBENZENE
	1-CHLORO-2,4-DINITROBENZENE
	1-Chloor-2,4-dinitrobenzeen
	1-Chlor-2,4-dinitrobenzene
	1-Chloro-2,4-dinitrobenzol
	1-Cloro-2,4-dinitrobenzene
	2,4-Dinitro-1-chlorobenzene
	2,4-Dinitrochlorobenzene
	2,4-Dinitrophenyl chloride
	4-Chloro-1,3-dinitrobenzene
	6-Chloro-1,3-dinitrobenzene
	CDNB
	DINITROCHLOROBENZENE
	DNCB
	Dinitrochlorobenzol
	NSC 6292
Inchi:	InChI=1S/C6H3ClN2O4/c7-5-2-1-4(8(10)11)3-6(5)9(12)13/h1-3H
InchiKey:	VYZAHLCBVHPDDF-UHFFFAOYSA-N
Formula:	C6H3ClN2O4
SMILES:	O=[N+]([O-])c1ccc(Cl)c([N+](=O)[O-])c1
Mol. weight [g/mol]:	202.55
CAS:	97-00-7

Physical Properties

Property code	Value	Unit	Source
gf	151.96	kJ/mol	Joback Method
hf	9.16	kJ/mol	Joback Method
hfus	31.48	kJ/mol	Joback Method
hvap	70.12	kJ/mol	Joback Method
log10ws	-3.46		Crippen Method
logp	2.156		Crippen Method
mcvol	118.720	ml/mol	McGowan Method
pc	4409.10	kPa	Joback Method
ripol	2526.00		NIST Webbook
ripol	2526.00		NIST Webbook
ripol	2545.00		NIST Webbook
tb	588.20	K	NIST Webbook

tc	997.45	K	Joback Method
tf	525.98	K	Joback Method
vc	0.476	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	290.51	J/mol×K	855.94	Joback Method
cpg	295.91	J/mol×K	903.11	Joback Method
cpg	300.65	J/mol×K	950.28	Joback Method
cpg	269.81	J/mol×K	714.43	Joback Method
cpg	277.51	J/mol×K	761.60	Joback Method
cpg	284.39	J/mol×K	808.77	Joback Method
cpg	304.79	J/mol×K	997.45	Joback Method
hfust	20.17	kJ/mol	325.20	NIST Webbook
hfust	20.20	kJ/mol	325.20	NIST Webbook
hvapt	80.50	kJ/mol	510.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.58470e+01
Coeff. B	-5.50759e+03
Coeff. C	-9.75060e+01
Temperature range (K), min.	451.48
Temperature range (K), max.	620.27

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	1.21700e+02
Coeff. B	-1.50568e+04
Coeff. C	-1.45454e+01
Coeff. D	3.65312e-06
Temperature range (K), min.	326.55

Temperature range (K), max.	813.77

Sources

KDB Vapor Pressure Data:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1793
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
Solubilities of Benzene Derivatives in Supercritical Carbon Dioxide:	https://www.doi.org/10.1021/je100863p
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C97007&Units=SI
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
KDB:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1793

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
hfust:	Enthalpy of fusion at a given temperature
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
pvap:	Vapor pressure
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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