Benzene, 4-methyl-1,2-dinitro-

Other names:	1-METHYL-3,4-DINTRO-BENZENE
	1-methyl-3,4-dinitrobenzene
	3,4-DINITROTOLUENE
	3,4-DNT
	Toluene, 3,4-dinitro-
	benzene, 1-methyl-3,4-dinitro-
Inchi:	InChI=1S/C7H6N2O4/c1-5-2-3-6(8(10)11)7(4-5)9(12)13/h2-4H,1H3
InchiKey:	INYDMNPNDHRJQJ-UHFFFAOYSA-N
Formula:	C7H6N2O4
SMILES:	Cc1ccc([N+](=O)[O-])c([N+](=O)[O-])c1
Mol. weight [g/mol]:	182.13
CAS:	610-39-9

Physical Properties

Property code	Value	Unit	Source
chs	-3598.00	kJ/mol	NIST Webbook
ea	1.77 ± 0.05	eV	NIST Webbook
gf	172.31	kJ/mol	Joback Method
hf	4.26	kJ/mol	Joback Method
hfus	29.87	kJ/mol	Joback Method
hvap	67.96	kJ/mol	Joback Method
log10ws	-3.25		Crippen Method
logp	1.811		Crippen Method
mcvol	120.570	ml/mol	McGowan Method
pc	4082.92	kPa	Joback Method
rinpol	1574.00		NIST Webbook
tb	699.88	K	Joback Method
tc	974.05	K	Joback Method
tf	329.00 ± 0.10	K	NIST Webbook
vc	0.483	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source

cpg	299.55	J/mol×K	699.88	Joback Method
cpg	309.27	J/mol×K	745.58	Joback Method
cpg	318.09	J/mol×K	791.27	Joback Method
cpg	326.05	J/mol×K	836.97	Joback Method
cpg	333.22	J/mol×K	882.66	Joback Method
cpg	339.64	J/mol×K	928.36	Joback Method
cpg	345.36	J/mol×K	974.05	Joback Method
hfust	18.83	kJ/mol	329.50	NIST Webbook
hfust	18.83	kJ/mol	329.50	NIST Webbook
hsubt	99.60 ± 1.90	kJ/mol	292.50	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.73159e+01
Coeff. B	-6.26733e+03
Coeff. C	-1.00075e+02
Temperature range (K), min.	468.13
Temperature range (K), max.	622.16

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	1.22011e+02
Coeff. B	-1.56000e+04
Coeff. C	-1.45153e+01
Coeff. D	3.38490e-06
Temperature range (K), min.	332.00
Temperature range (K), max.	842.00

Sources

Joback Method: https://en.wikipedia.org/wiki/Joback_method

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C610399&Units=SI

The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Solubility of 3,4-Dinitrotoluene in Pure Water and Seawater:	https://www.doi.org/10.1021/je700520k
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
KDB Vapor Pressure Data:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1448
KDB:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1448

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
hfus:	Enthalpy of fusion at standard conditions
hfust:	Enthalpy of fusion at a given temperature
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
pvap:	Vapor pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume