Benzene, 1-methyl-3,5-dinitro-

Other names:	1-METHYL-3,5-DINTRO-BENZENE
	1-Methyl-3,5-dinitrobenzene
	3,5-DINITROTOLUENE
	3,5-DNT
	Toluene, 3,5-dinitro-
Inchi:	InChI=1S/C7H6N2O4/c1-5-2-6(8(10)11)4-7(3-5)9(12)13/h2-4H,1H3
InchiKey:	RUIFULUFLANOCI-UHFFFAOYSA-N
Formula:	C7H6N2O4
SMILES:	Cc1cc([N+](=O)[O-])cc([N+](=O)[O-])c1
Mol. weight [g/mol]:	182.13
CAS:	618-85-9

Physical Properties

Property code	Value	Unit	Source
chs	-3569.00	kJ/mol	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
tb	699.88	K	Joback Method
tc	974.05	K	Joback Method
tf	507.33	K	Joback Method
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
hvapt	62.60	kJ/mol	518.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.66884e+01
Coeff. B	-6.87757e+03
Coeff. C	-2.12820e+01
Temperature range (K), min.	440.63
Temperature range (K), max.	625.80

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	4.65523e+01
Coeff. B	-9.30483e+03
Coeff. C	-4.17683e+00
Coeff. D	1.51050e-06
Temperature range (K), min.	365.65
Temperature range (K), max.	814.00

Sources

The Yaws Handbook of Vapor Pressure: https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
KDB Vapor Pressure Data: https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1449
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method: https://en.wikipedia.org/wiki/Joback_method
KDB: https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1449
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C618859&Units=SI

Legend

chs:	Standard solid enthalpy of combustion
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
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume