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

Other names:	1-Methyl-2,4-Dinitrobenzene
	2,4-DNT
	2,4-Dinitrotoluene
	2,4-Dinitrotoluol
	4-Methyl-1,3-dinitrobenzene
	6-Methyl-1,3-dinitrobenzene
	Dinitrotoluol
	NCI-C01865
	NSC 7194
	Rcra waste number U105
	Toluene, 2,4-dinitro-
Inchi:	InChI=1S/C7H6N2O4/c1-5-2-3-6(8(10)11)4-7(5)9(12)13/h2-4H,1H3
InchiKey:	RMBFBMJGBANMMK-UHFFFAOYSA-N
Formula:	C7H6N2O4
SMILES:	Cc1ccc([N+](=O)[O-])cc1[N+](=O)[O-]
Mol. weight [g/mol]:	182.13
CAS:	121-14-2

Physical Properties

Property code	Value	Unit	Source
ea	1.60 ± 0.05	eV	NIST Webbook
gf	172.31	kJ/mol	Joback Method
hf	33.20 ± 3.30	kJ/mol	NIST Webbook
hfs	-66.40 ± 3.00	kJ/mol	NIST Webbook
hfs	-40.00	kJ/mol	NIST Webbook
hfs	-29.00	kJ/mol	NIST Webbook
hfus	29.87	kJ/mol	Joback Method
hsub	99.60 ± 2.50	kJ/mol	NIST Webbook
hsub	100.00 ± 1.00	kJ/mol	NIST Webbook
hvap	67.96	kJ/mol	Joback Method
log10ws	-2.82		Estimated Solubility Method
log10ws	-2.82		Aqueous Solubility Prediction Method
logp	1.811		Crippen Method
mcvol	120.570	ml/mol	McGowan Method
pc	4082.92	kPa	Joback Method

rinpol	1537.00		NIST Webbook
rinpol	1549.11		NIST Webbook
rinpol	261.80		NIST Webbook
rinpol	262.61		NIST Webbook
rinpol	1537.00		NIST Webbook
rinpol	1497.00		NIST Webbook
rinpol	1550.09		NIST Webbook
rinpol	1497.00		NIST Webbook
rinpol	1537.00		NIST Webbook
rinpol	1531.81		NIST Webbook
rinpol	1541.10		NIST Webbook
rinpol	1498.00		NIST Webbook
rinpol	1549.11		NIST Webbook
ripol	2420.00		NIST Webbook
ripol	2420.00		NIST Webbook
ripol	2420.00		NIST Webbook
tb	699.88	K	Joback Method
tc	974.05	K	Joback Method
tf	345.00 ± 1.00	K	NIST Webbook
tf	340.00 ± 1.00	K	NIST Webbook
tf	343.00 ± 1.50	K	NIST Webbook
tf	344.30 ± 0.50	K	NIST Webbook
tf	341.00 ± 0.10	K	NIST Webbook
tf	342.53	K	Aqueous Solubility Prediction Method
vc	0.483	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	339.64	J/mol×K	928.36	Joback Method
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	345.36	J/mol×K	974.05	Joback Method
cps	255.00	J/mol×K	325.00	NIST Webbook
hfust	20.90	kJ/mol	345.00	NIST Webbook
hfust	20.12	kJ/mol	343.30	NIST Webbook
hfust	20.12	kJ/mol	343.30	NIST Webbook

hsubt	95.80 ± 1.30	kJ/mol	310.50	NIST Webbook
hsubt	94.70 ± 2.30	kJ/mol	292.50	NIST Webbook
hsubt	98.30 ± 2.50	kJ/mol	337.00	NIST Webbook
hvapt	70.20	kJ/mol	396.50	NIST Webbook
hvapt	76.90	kJ/mol	458.00	NIST Webbook
hvapt	58.20	kJ/mol	522.50	NIST Webbook
psub	3.16e-03	kPa	338.15	Triacetone triperoxide thermogravimetric study of vapor pressure and enthalpy of sublimation in 303 338 K temperature range
psub	1.01e-04	kPa	308.15	Triacetone triperoxide thermogravimetric study of vapor pressure and enthalpy of sublimation in 303 338 K temperature range
psub	1.98e-04	kPa	313.15	Triacetone triperoxide thermogravimetric study of vapor pressure and enthalpy of sublimation in 303 338 K temperature range
psub	3.69e-04	kPa	318.15	Triacetone triperoxide thermogravimetric study of vapor pressure and enthalpy of sublimation in 303 338 K temperature range
psub	6.67e-04	kPa	323.15	Triacetone triperoxide thermogravimetric study of vapor pressure and enthalpy of sublimation in 303 338 K temperature range

psub	1.16e-03	kPa	328.15	Triacetone triperoxide thermogravimetric study of vapor pressure and enthalpy of sublimation in 303 338 K temperature range
psub	1.97e-03	kPa	333.15	Triacetone triperoxide thermogravimetric study of vapor pressure and enthalpy of sublimation in 303 338 K temperature range
sfust	61.00	J/mol×K	345.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.78315e+01
Coeff. B	-8.56181e+03
Coeff. C	5.33810e+01
Temperature range (K), min.	434.64
Temperature range (K), max.	630.47

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	1.43080e+01
Coeff. B	-6.62964e+03
Coeff. C	1.74908e-01
Coeff. D	1.20512e-06
Temperature range (K), min.	343.00
Temperature range (K), max.	814.00

Sources

KDB Vapor Pressure Data:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1445
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Triacetone triperoxide thermogravimetric study of vapor pressure and enthalpy of sublimation in 303 338 K temperature range:	https://www.doi.org/10.1016/j.tca.2010.11.034
Estimated Solubility Method:	http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt
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
KDB:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1445
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C121142&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

cpg:	Ideal gas heat capacity
cps:	Solid phase heat capacity
ea:	Electron affinity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfs:	Solid phase enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hfust:	Enthalpy of fusion at a given temperature
hsub:	Enthalpy of sublimation at standard conditions
hsubt:	Enthalpy of sublimation 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
psub:	Sublimation pressure
pvap:	Vapor pressure
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
sfust:	Entropy of fusion at a given temperature
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point

vc: Critical Volume