Benzene, 2-methyl-1,3-dinitro-

Other names:	1-Methyl-2,6-dinitrobenzene
	2,6-DNT (2,6-dinitrotoluene)
	2,6-Dinitrotoluene
	2,6-Dnt
	2-Methyl-1,3-dinitro-benzene
	2-methyl-1,3-dinitrobenzene
	Rcra waste number U106
	Toluene, 2,6-dinitro-
Inchi:	InChI=1S/C7H6N2O4/c1-5-6(8(10)11)3-2-4-7(5)9(12)13/h2-4H,1H3
InchiKey:	XTRDKALNCIHHNI-UHFFFAOYSA-N
Formula:	C7H6N2O4
SMILES:	Cc1c([N+](=O)[O-])cccc1[N+](=O)[O-]
Mol. weight [g/mol]:	182.13
CAS:	606-20-2

Physical Properties

Property code	Value	Unit	Source
chs	-3574.00	kJ/mol	NIST Webbook
chs	-3560.90 ± 3.60	kJ/mol	NIST Webbook
chs	-3570.30	kJ/mol	NIST Webbook
chs	-3556.80 ± 1.00	kJ/mol	NIST Webbook
ea	1.55 ± 0.05	eV	NIST Webbook
ea	1.47 ± 0.05	eV	NIST Webbook
gf	172.31	kJ/mol	Joback Method
hf	4.26	kJ/mol	Joback Method
hfs	-41.80	kJ/mol	NIST Webbook
hfs	-55.20 ± 2.20	kJ/mol	NIST Webbook
hfus	29.87	kJ/mol	Joback Method
hvap	67.96	kJ/mol	Joback Method
log10ws	-3.00		Aqueous Solubility Prediction Method
log10ws	-3.00		Estimated Solubility Method
logp	1.811		Crippen Method
mcvol	120.570	ml/mol	McGowan Method
pc	4082.92	kPa	Joback Method
rinpol	250.87		NIST Webbook

rinpol	1392.00		NIST Webbook
rinpol	1392.00		NIST Webbook
rinpol	1385.00		NIST Webbook
rinpol	1415.00		NIST Webbook
rinpol	250.00		NIST Webbook
rinpol	1416.00		NIST Webbook
rinpol	1385.00		NIST Webbook
rinpol	1401.00		NIST Webbook
ripol	2322.00		NIST Webbook
ripol	2322.00		NIST Webbook
tb	699.88	K	Joback Method
tc	974.05	K	Joback Method
tf	339.00 ± 3.00	K	NIST Webbook
tf	327.00 ± 0.10	K	NIST Webbook
tf	339.19 ± 0.10	K	NIST Webbook
tf	329.60 ± 0.20	K	NIST Webbook
tf	337.65	K	Aqueous Solubility Prediction Method
vc	0.483	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
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	299.55	J/mol×K	699.88	Joback Method
cpg	345.36	J/mol×K	974.05	Joback Method
cps	217.00	J/mol×K	305.00	NIST Webbook
cps	224.00	J/mol×K	305.00	NIST Webbook
hfust	23.85	kJ/mol	327.50	NIST Webbook
hfust	16.07	kJ/mol	340.00	NIST Webbook
hfust	19.28	kJ/mol	340.00	NIST Webbook
hfust	23.85	kJ/mol	327.50	NIST Webbook
hsubt	98.30 ± 0.80	kJ/mol	300.00	NIST Webbook
hsubt	99.60 ± 2.30	kJ/mol	300.00	NIST Webbook
hvapt	68.70	kJ/mol	385.50	NIST Webbook
hvapt	56.90	kJ/mol	488.00	NIST Webbook
hvapt	77.80	kJ/mol	431.50	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.46496e+01
Coeff. B	-4.86051e+03
Coeff. C	-9.13380e+01
Temperature range (K), min.	429.77
Temperature range (K), max.	611.84

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	2.82485e+02
Coeff. B	-2.25355e+04
Coeff. C	-3.83779e+01
Coeff. D	1.69581e-05
Temperature range (K), min.	339.00
Temperature range (K), max.	770.00

Sources

KDB Vapor Pressure Data:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1447
KDB:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1447
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C606202&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
Solubility of 4-Nitrotoluene, 2,6-Dinitrotoluene, 2,3-Dinitrotoluene, and 1,3,5-Trinitrobenzene in Pure Water and Seawater:	https://www.doi.org/10.1021/je700374j
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
Estimated Solubility Method:	http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

chs:	Standard solid enthalpy of combustion
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
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
pvap:	Vapor pressure
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume