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

Other names:	1-Methyl-2,3-dinitro-benzene
	1-methyl-2,3-dinitrobenzene
	2,3-DNT
	2,3-dinitrotoluene
	toluene, 2,3-dinitro-
Inchi:	InChI=1S/C7H6N2O4/c1-5-3-2-4-6(8(10)11)7(5)9(12)13/h2-4H,1H3
InchiKey:	DYSXLQBUUOPLBB-UHFFFAOYSA-N
Formula:	C7H6N2O4
SMILES:	Cc1cccc([N+](=O)[O-])c1[N+](=O)[O-]
Mol. weight [g/mol]:	182.13
CAS:	602-01-7

Physical Properties

Property code	Value	Unit	Source
chs	-4015.00	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
tb	699.88	K	Joback Method
tc	974.05	K	Joback Method
tf	330.00 ± 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	17.57	kJ/mol	329.80	NIST Webbook
hfust	17.57	kJ/mol	329.80	NIST Webbook
hsubt	97.00 ± 2.10	kJ/mol	292.50	NIST Webbook

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C602017&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
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

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume