

# Benzenamine, 2-methyl-3,5-dinitro-

<b>Other names:</b>	2-Amino-4,6-dinitrotoluene 2,4-Dinitro-6-aminotoluene 3,5-Dinitro-o-toluidine 2-Methyl-3,5-dinitroaniline o-Toluidine, 3,5-dinitro- 2-Adnt 2-Methyl-3,5-dinitrobenzenamine
<b>Inchi:</b>	InChI=1S/C7H7N3O4/c1-4-6(8)2-5(9(11)12)3-7(4)10(13)14/h2-3H,8H2,1H3
<b>InchiKey:</b>	IEEJAAUSLQCGJH-UHFFFAOYSA-N
<b>Formula:</b>	C7H7N3O4
<b>SMILES:</b>	<chem>Cc1c(N)cc([N+](=O)[O-])cc1[N+](=O)[O-]</chem>
<b>Mol. weight [g/mol]:</b>	197.15
<b>CAS:</b>	35572-78-2

## Physical Properties

Property code	Value	Unit	Source
gf	229.13	kJ/mol	Joback Method
hf	26.58	kJ/mol	Joback Method
hfus	34.68	kJ/mol	Joback Method
hvap	79.26	kJ/mol	Joback Method
log10ws	-2.88		Crippen Method
logp	1.394		Crippen Method
mvol	130.550	ml/mol	McGowan Method
pc	4311.22	kPa	Joback Method
rinpol	330.74		NIST Webbook
rinpol	330.74		NIST Webbook
tb	777.39	K	Joback Method
tc	1055.29	K	Joback Method
tf	603.11	K	Joback Method
vc	0.512	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
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cpg	345.91	J/mol×K	777.39	Joback Method
cpg	354.86	J/mol×K	823.71	Joback Method
cpg	362.94	J/mol×K	870.02	Joback Method
cpg	370.17	J/mol×K	916.34	Joback Method
cpg	376.61	J/mol×K	962.66	Joback Method
cpg	382.30	J/mol×K	1008.97	Joback Method
cpg	387.28	J/mol×K	1055.29	Joback Method

## Sources

<b>McGowan Method:</b>	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C35572782&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C35572782&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</a>
<b>Crippen Method:</b>	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>
<b>Joback Method:</b>	<a href="https://en.wikipedia.org/wiki/Joback_method">https://en.wikipedia.org/wiki/Joback_method</a>

## Legend

<b>cpg:</b>	Ideal gas heat capacity
<b>gf:</b>	Standard Gibbs free energy of formation
<b>hf:</b>	Enthalpy of formation at standard conditions
<b>hfus:</b>	Enthalpy of fusion at standard conditions
<b>hvap:</b>	Enthalpy of vaporization at standard conditions
<b>log10ws:</b>	Log10 of Water solubility in mol/l
<b>logp:</b>	Octanol/Water partition coefficient
<b>mcvol:</b>	McGowan's characteristic volume
<b>pc:</b>	Critical Pressure
<b>rinpol:</b>	Non-polar retention indices
<b>tb:</b>	Normal Boiling Point Temperature
<b>tc:</b>	Critical Temperature
<b>tf:</b>	Normal melting (fusion) point
<b>vc:</b>	Critical Volume

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