

# Benzenamine, 2,4,6-trinitro-

<b>Other names:</b>	Aniline, 2,4,6-trinitro- Picramide 2,4,6-Trinitroaniline
<b>Inchi:</b>	InChI=1S/C6H4N4O6/c7-6-4(9(13)14)1-3(8(11)12)2-5(6)10(15)16/h1-2H,7H2
<b>InchiKey:</b>	IAHOUQOWMXVMEH-UHFFFAOYSA-N
<b>Formula:</b>	C6H4N4O6
<b>SMILES:</b>	Nc1c([N+](=O)[O-])cc([N+](=O)[O-])cc1[N+](=O)[O-]
<b>Mol. weight [g/mol]:</b>	228.12
<b>CAS:</b>	489-98-5

## Physical Properties

Property code	Value	Unit	Source
chs	-2860.10	kJ/mol	NIST Webbook
chs	-2816.87	kJ/mol	NIST Webbook
gf	256.26	kJ/mol	Joback Method
hf	36.46	kJ/mol	Joback Method
hfs	-115.90	kJ/mol	NIST Webbook
hfs	-72.80	kJ/mol	NIST Webbook
hfus	43.45	kJ/mol	Joback Method
hsub	125.30 ± 0.80	kJ/mol	NIST Webbook
hvap	93.63	kJ/mol	Joback Method
log10ws	-3.06		Crippen Method
logp	0.993		Crippen Method
mcvol	133.880	ml/mol	McGowan Method
pc	4994.44	kPa	Joback Method
rinpol	337.56		NIST Webbook
tb	906.35	K	Joback Method
tc	1204.38	K	Joback Method
tf	735.45	K	Joback Method
vc	0.538	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
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cpg	365.18	J/mol×K	906.35	Joback Method
cpg	371.25	J/mol×K	956.02	Joback Method
cpg	376.44	J/mol×K	1005.69	Joback Method
cpg	380.82	J/mol×K	1055.37	Joback Method
cpg	384.44	J/mol×K	1105.04	Joback Method
cpg	387.36	J/mol×K	1154.71	Joback Method
cpg	389.64	J/mol×K	1204.38	Joback Method
hsubt	115.90	kJ/mol	349.50	NIST Webbook

## Sources

Crippen Method:	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307l">http://pubs.acs.org/doi/abs/10.1021/ci990307l</a>
Crippen Method:	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>
Joback Method:	<a href="https://en.wikipedia.org/wiki/Joback_method">https://en.wikipedia.org/wiki/Joback_method</a>
McGowan Method:	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>
NIST Webbook:	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C489985&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C489985&amp;Units=SI</a>

## Legend

<b>chs:</b>	Standard solid enthalpy of combustion
<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>hfs:</b>	Solid phase enthalpy of formation at standard conditions
<b>hfus:</b>	Enthalpy of fusion at standard conditions
<b>hsub:</b>	Enthalpy of sublimation at standard conditions
<b>hsubt:</b>	Enthalpy of sublimation at a given temperature
<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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