

# Benzoic acid, 2,4,6-trinitro-

<b>Other names:</b>	s-Trinitrobenzoic acid Benzoic acid, trinitro- (dry) Benzoic acid, trinitro- (wet) Trinitrobenzoic acid 2,4,6-Trinitrobenzoic acid Benzoic acid, trinitro- NSC 133453 sym-Trinitrobenzoic acid
<b>Inchi:</b>	InChI=1S/C7H3N3O8/c11-7(12)6-4(9(15)16)1-3(8(13)14)2-5(6)10(17)18/h1-2H,(H,11,12)
<b>InchiKey:</b>	KAQBNBSMMVTKRN-UHFFFAOYSA-N
<b>Formula:</b>	C7H3N3O8
<b>SMILES:</b>	O=C(O)c1c([N+](=O)[O-])cc([N+](=O)[O-])cc1[N+](=O)[O-]
<b>Mol. weight [g/mol]:</b>	257.11
<b>CAS:</b>	129-66-8

## Physical Properties

Property code	Value	Unit	Source
chs	-2773.70	kJ/mol	NIST Webbook
gf	-67.51	kJ/mol	Joback Method
hf	-282.78	kJ/mol	Joback Method
hfs	-409.70	kJ/mol	NIST Webbook
hfus	46.53	kJ/mol	Joback Method
hvap	108.64	kJ/mol	Joback Method
log10ws	-3.48		Crippen Method
logp	1.109		Crippen Method
mcvol	145.430	ml/mol	McGowan Method
pc	5008.59	kPa	Joback Method
tb	1002.75	K	Joback Method
tc	1270.35	K	Joback Method
tf	774.21	K	Joback Method
vc	0.591	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	399.46	J/mol×K	1002.75	Joback Method
cpg	403.37	J/mol×K	1047.35	Joback Method
cpg	406.59	J/mol×K	1091.95	Joback Method
cpg	409.17	J/mol×K	1136.55	Joback Method
cpg	411.15	J/mol×K	1181.15	Joback Method
cpg	412.57	J/mol×K	1225.75	Joback Method
cpg	413.48	J/mol×K	1270.35	Joback Method

## Sources

<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>
<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=C129668&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C129668&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>

## 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>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>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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