

# 1,3,5-Triazine-2,4,6(1H,3H,5H)-trione, 1,3,5-trimethyl-

<b>Other names:</b>	s-Triazine-2,4,6(1H,3H,5H)-trione, 1,3,5-trimethyl- Isocyanuric acid, trimethyl ester Methyl isocyanate trimer Trimethyl isocyanurate 1,3,5-Trimethyl-2,4,6-trioxohexahydrotriazine
<b>Inchi:</b>	InChI=1S/C6H9N3O3/c1-7-4(10)8(2)6(12)9(3)5(7)11/h1-3H3
<b>InchiKey:</b>	AHWDQDMGFXRFB-UHFFFAOYSA-N
<b>Formula:</b>	C6H9N3O3
<b>SMILES:</b>	Cn1c(=O)n(C)c(=O)n(C)c1=O
<b>Mol. weight [g/mol]:</b>	171.15
<b>CAS:</b>	827-16-7

## Physical Properties

Property code	Value	Unit	Source
chs	-2968.59 ± 0.49	kJ/mol	NIST Webbook
hf	-590.50 ± 1.60	kJ/mol	NIST Webbook
hfs	-678.70 ± 1.00	kJ/mol	NIST Webbook
hsub	88.20 ± 1.20	kJ/mol	NIST Webbook
log10ws	-3.60		Crippen Method
logp	-2.217		Crippen Method
mcvol	119.190	ml/mol	McGowan Method
tb	547.20	K	NIST Webbook

## 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=C827167&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C827167&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>

# Legend

<b>chs:</b>	Standard solid enthalpy of combustion
<b>hf:</b>	Enthalpy of formation at standard conditions
<b>hfs:</b>	Solid phase enthalpy of formation at standard conditions
<b>hsub:</b>	Enthalpy of sublimation 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>tb:</b>	Normal Boiling Point Temperature

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