

# 1,1,1-Trinitro-2-ethoxypropane

<b>Inchi:</b>	InChI=1S/C5H9N3O7/c1-3-15-4(2)5(6(9)10,7(11)12)8(13)14/h4H,3H2,1-2H3
<b>InchiKey:</b>	HTKFMBXRRYDJDL-UHFFFAOYSA-N
<b>Formula:</b>	C5H9N3O7
<b>SMILES:</b>	CCOC(C)C([N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-]
<b>Mol. weight [g/mol]:</b>	223.14
<b>CAS:</b>	26459-85-8

## Physical Properties

Property code	Value	Unit	Source
gf	-6.73	kJ/mol	Joback Method
hf	-325.06	kJ/mol	Joback Method
hfus	33.04	kJ/mol	Joback Method
hvap	77.22	kJ/mol	Joback Method
log10ws	-2.47		Crippen Method
logp	-0.105		Crippen Method
mcvol	139.440	ml/mol	McGowan Method
pc	3664.21	kPa	Joback Method
tb	788.07	K	Joback Method
tc	1055.12	K	Joback Method
tf	586.59	K	Joback Method
vc	0.562	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	401.28	J/molxK	788.07	Joback Method
cpg	410.33	J/molxK	832.58	Joback Method
cpg	418.43	J/molxK	877.09	Joback Method
cpg	425.66	J/molxK	921.60	Joback Method
cpg	432.09	J/molxK	966.11	Joback Method
cpg	437.77	J/molxK	1010.61	Joback Method
cpg	442.78	J/molxK	1055.12	Joback Method

# Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C26459858&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C26459858&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>
<b>McGowan Method:</b>	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</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>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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