

# Ethane, 1,1,1-trimethoxy-

<b>Other names:</b>	Orthoacetic acid, trimethyl ester Methyl orthoacetate Trimethyl orthoacetate 1,1,1-Trimethoxyethane CH <sub>3</sub> C(OCH <sub>3</sub> ) <sub>3</sub>
<b>Inchi:</b>	InChI=1S/C5H12O3/c1-5(6-2,7-3)8-4/h1-4H3
<b>InchiKey:</b>	HDPNBNXLBDFELL-UHFFFAOYSA-N
<b>Formula:</b>	C <sub>5</sub> H <sub>12</sub> O <sub>3</sub>
<b>SMILES:</b>	COC(C)(OC)OC
<b>Mol. weight [g/mol]:</b>	120.15
<b>CAS:</b>	1445-45-0

## Physical Properties

Property code	Value	Unit	Source
gf	-320.94	kJ/mol	Joback Method
hf	-572.70 ± 2.30	kJ/mol	NIST Webbook
hf	-570.86 ± 0.87	kJ/mol	NIST Webbook
hfl	-610.00 ± 0.45	kJ/mol	NIST Webbook
hfl	-612.00 ± 1.10	kJ/mol	NIST Webbook
hfus	4.86	kJ/mol	Joback Method
hvap	39.30	kJ/mol	NIST Webbook
hvap	39.10	kJ/mol	NIST Webbook
hvap	39.20	kJ/mol	NIST Webbook
hvap	39.20 ± 0.75	kJ/mol	NIST Webbook
ie	9.65	eV	NIST Webbook
log10ws	-0.28		Crippen Method
logp	0.599		Crippen Method
mvol	98.920	ml/mol	McGowan Method
pc	3341.24	kPa	Joback Method
tb	381.20	K	NIST Webbook
tc	555.11	K	Joback Method
tf	215.22	K	Joback Method
vc	0.358	m <sup>3</sup> /kmol	Joback Method

# Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	192.40	J/molxK	377.83	Joback Method
cpg	202.04	J/molxK	407.38	Joback Method
cpg	211.43	J/molxK	436.92	Joback Method
cpg	220.57	J/molxK	466.47	Joback Method
cpg	229.46	J/molxK	496.01	Joback Method
cpg	238.07	J/molxK	525.56	Joback Method
cpg	246.41	J/molxK	555.11	Joback Method
dvisc	0.0033768	Paxs	215.22	Joback Method
dvisc	0.0016415	Paxs	242.32	Joback Method
dvisc	0.0009226	Paxs	269.42	Joback Method
dvisc	0.0005761	Paxs	296.52	Joback Method
dvisc	0.0003893	Paxs	323.63	Joback Method
dvisc	0.0002795	Paxs	350.73	Joback Method
dvisc	0.0002104	Paxs	377.83	Joback Method

## Sources

<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>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C1445450&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C1445450&amp;Units=SI</a>

## Legend

<b>cpg:</b>	Ideal gas heat capacity
<b>dvisc:</b>	Dynamic viscosity
<b>gf:</b>	Standard Gibbs free energy of formation
<b>hf:</b>	Enthalpy of formation at standard conditions
<b>hfl:</b>	Liquid 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>ie:</b>	Ionization energy

<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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