

# 1,1,3-triethoxyhexane

<b>Inchi:</b>	InChI=1S/C12H26O3/c1-5-9-11(13-6-2)10-12(14-7-3)15-8-4/h11-12H,5-10H2,1-4H3
<b>InchiKey:</b>	SYPLTTUVUZHTJR-UHFFFAOYSA-N
<b>Formula:</b>	C12H26O3
<b>SMILES:</b>	CCCC(CC(OCC)OCC)OCC
<b>Mol. weight [g/mol]:</b>	218.33
<b>CAS:</b>	101-33-7

## Physical Properties

Property code	Value	Unit	Source
gf	-269.72	kJ/mol	Joback Method
hf	-698.23	kJ/mol	Joback Method
hfus	23.35	kJ/mol	Joback Method
hvap	48.76	kJ/mol	Joback Method
log10ws	-2.83		Crippen Method
logp	2.981		Crippen Method
mcvol	197.550	ml/mol	McGowan Method
pc	1728.90	kPa	Joback Method
tb	540.34	K	Joback Method
tc	707.13	K	Joback Method
tf	173.15	K	NIST Webbook
vc	0.750	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	493.50	J/molxK	540.34	Joback Method
cpg	510.18	J/molxK	568.14	Joback Method
cpg	526.29	J/molxK	595.94	Joback Method
cpg	541.84	J/molxK	623.73	Joback Method
cpg	556.83	J/molxK	651.53	Joback Method
cpg	571.25	J/molxK	679.33	Joback Method
cpg	585.10	J/molxK	707.13	Joback Method
dvisc	0.0041810	Paxs	261.69	Joback Method
dvisc	0.0014140	Paxs	308.13	Joback Method

dvisc	0.0006353	Paxs	354.57	Joback Method
dvisc	0.0003435	Paxs	401.01	Joback Method
dvisc	0.0002111	Paxs	447.46	Joback Method
dvisc	0.0001421	Paxs	493.90	Joback Method
dvisc	0.0001024	Paxs	540.34	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=C101337&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C101337&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>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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