

# cis-1,3,5-Cyclohexanetricarboxylic acid, triethyl ester

Inchi:	InChI=1S/C15H24O6/c1-4-19-13(16)10-7-11(14(17)20-5-2)9-12(8-10)15(18)21-6-3/h10-1
InchiKey:	JQFXPGZFIFHJJV-ZSBIGDGJSA-N
Formula:	C15H24O6
SMILES:	CCOC(=O)C1CC(C(=O)OCC)CC(C(=O)OCC)C1
Mol. weight [g/mol]:	300.35

## Physical Properties

Property code	Value	Unit	Source
gf	-617.31	kJ/mol	Joback Method
hf	-1073.69	kJ/mol	Joback Method
hfus	36.94	kJ/mol	Joback Method
hvap	76.26	kJ/mol	Joback Method
log10ws	-1.86		Crippen Method
logp	1.708		Crippen Method
mcvol	233.670	ml/mol	McGowan Method
pc	1763.93	kPa	Joback Method
rinpol	1972.00		NIST Webbook
rinpol	1972.00		NIST Webbook
tb	781.68	K	Joback Method
tc	985.04	K	Joback Method
tf	474.19	K	Joback Method
vc	0.878	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	729.14	J/molxK	781.68	Joback Method
cpg	799.82	J/molxK	951.15	Joback Method
cpg	788.27	J/molxK	917.25	Joback Method
cpg	775.40	J/molxK	883.36	Joback Method
cpg	761.25	J/molxK	849.47	Joback Method
cpg	745.83	J/molxK	815.57	Joback Method
cpg	810.05	J/molxK	985.04	Joback Method
dvisc	0.0001288	Paxs	781.68	Joback Method

dvisc	0.0001606	Paxs	730.43	Joback Method
dvisc	0.0002069	Paxs	679.18	Joback Method
dvisc	0.0002780	Paxs	627.93	Joback Method
dvisc	0.0003936	Paxs	576.69	Joback Method
dvisc	0.0005963	Paxs	525.44	Joback Method
dvisc	0.0009883	Paxs	474.19	Joback Method

## Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=R96404&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R96404&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>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>rinpol:</b>	Non-polar retention indices
<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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