

# Glutaric acid, ethyl non-5-yn-3-yl ester

<b>Inchi:</b>	InChI=1S/C16H26O4/c1-4-7-8-9-11-14(5-2)20-16(18)13-10-12-15(17)19-6-3/h14H,4-7,10
<b>InchiKey:</b>	BMDUHDYSZROBHT-UHFFFAOYSA-N
<b>Formula:</b>	C16H26O4
<b>SMILES:</b>	CCCC#CCC(CC)OC(=O)CCCC(=O)OCC
<b>Mol. weight [g/mol]:</b>	282.38

## Physical Properties

Property code	Value	Unit	Source
gf	-183.64	kJ/mol	Joback Method
hf	-596.15	kJ/mol	Joback Method
hfus	42.37	kJ/mol	Joback Method
hvap	71.29	kJ/mol	Joback Method
log10ws	-4.15		Crippen Method
logp	3.235		Crippen Method
mcvol	242.580	ml/mol	McGowan Method
pc	1607.71	kPa	Joback Method
rinpola	1920.00		NIST Webbook
tb	726.62	K	Joback Method
tc	918.00	K	Joback Method
tf	505.50	K	Joback Method
vc	0.935	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	688.55	J/mol×K	726.62	Joback Method
cpg	704.73	J/mol×K	758.52	Joback Method
cpg	720.03	J/mol×K	790.41	Joback Method
cpg	734.46	J/mol×K	822.31	Joback Method
cpg	748.04	J/mol×K	854.21	Joback Method
cpg	760.75	J/mol×K	886.10	Joback Method
cpg	772.61	J/mol×K	918.00	Joback Method

# Sources

<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=U359797&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U359797&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307l">http://pubs.acs.org/doi/abs/10.1021/ci990307l</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>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>hvac:</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>mccvol:</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

Latest version available from:

<https://www.chemeo.com/cid/32-855-7/Glutaric-acid-ethyl-non-5-yn-3-yl-ester.pdf>

Generated by Cheméo on 2024-05-01 03:23:47.52864574 +0000 UTC m=+16823076.449223051.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.