

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

**Inchi:** InChI=1S/C32H58O4/c1-4-7-9-11-12-13-14-15-16-17-18-19-20-21-22-24-29-35-31(33)27  
**InchiKey:** MHMQADCCAYHXNJ-UHFFFAOYSA-N  
**Formula:** C32H58O4  
**SMILES:** CCCC#CCC(CC)OC(=O)CCCC(=O)OCCCCCCCCCCCCCCCCCC  
**Mol. weight [g/mol]:** 506.80

## Physical Properties

Property code	Value	Unit	Source
gf	-48.92	kJ/mol	Joback Method
hf	-926.39	kJ/mol	Joback Method
hfus	83.81	kJ/mol	Joback Method
hvap	106.90	kJ/mol	Joback Method
log10ws	-10.85		Crippen Method
logp	9.477		Crippen Method
mcvol	468.020	ml/mol	McGowan Method
pc	615.73	kPa	Joback Method
rinpol	3560.00		NIST Webbook
rinpol	3560.00		NIST Webbook
tb	1092.70	K	Joback Method
tc	1372.32	K	Joback Method
tf	685.82	K	Joback Method
vc	1.831	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1678.25	J/mol×K	1092.70	Joback Method
cpg	1700.92	J/mol×K	1139.30	Joback Method
cpg	1720.91	J/mol×K	1185.91	Joback Method
cpg	1738.36	J/mol×K	1232.51	Joback Method
cpg	1753.41	J/mol×K	1279.11	Joback Method
cpg	1766.18	J/mol×K	1325.72	Joback Method
cpg	1776.82	J/mol×K	1372.32	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=U359815&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U359815&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307I">http://pubs.acs.org/doi/abs/10.1021/ci990307I</a>
<b>Crippen Method:</b>	<a href="https://www.cheméo.com/doc/models/crippen_log10ws">https://www.cheméo.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>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>rlnpol:</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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