

# Glutaric acid, 2,7-dimethyloct-5-yn-7-en-4-yl heptadecyl ester

<b>Inchi:</b>	InChI=1S/C32H56O4/c1-6-7-8-9-10-11-12-13-14-15-16-17-18-19-20-26-35-31(33)22-21-
<b>InchiKey:</b>	LPDTVYUDPRLXGA-UHFFFAOYSA-N
<b>Formula:</b>	C32H56O4
<b>SMILES:</b>	<chem>C=C(C)C#CC(CC(C)C)OC(=O)CCCC(=O)OCCCCCCCCCCCCCCCCCC</chem>
<b>Mol. weight [g/mol]:</b>	504.78

## Physical Properties

Property code	Value	Unit	Source
gf	27.93	kJ/mol	Joback Method
hf	-816.03	kJ/mol	Joback Method
hfus	77.70	kJ/mol	Joback Method
hvap	105.92	kJ/mol	Joback Method
log10ws	-10.46		Crippen Method
logp	9.109		Crippen Method
mvol	463.720	ml/mol	McGowan Method
pc	632.89	kPa	Joback Method
rmpol	3387.00		NIST Webbook
tb	1088.82	K	Joback Method
tc	1357.47	K	Joback Method
tf	655.10	K	Joback Method
vc	1.808	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1646.91	J/molxK	1088.82	Joback Method
cpg	1668.59	J/molxK	1133.60	Joback Method
cpg	1687.94	J/molxK	1178.37	Joback Method
cpg	1705.07	J/molxK	1223.15	Joback Method
cpg	1720.12	J/molxK	1267.92	Joback Method
cpg	1733.22	J/molxK	1312.70	Joback Method
cpg	1744.49	J/molxK	1357.47	Joback Method

# Sources

<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>
<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=U359850&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U359850&amp;Units=SI</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>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

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