

# Glutaric acid, 2,6-dimethylnon-1-en-3-yn-5-yl undecyl ester

**Inchi:** InChI=1S/C27H46O4/c1-6-8-9-10-11-12-13-14-15-22-30-26(28)18-16-19-27(29)31-25(21)  
**InchiKey:** DDQLKVUTLIDFPQ-UHFFFAOYSA-N  
**Formula:** C27H46O4  
**SMILES:** C=C(C)C#CC(OC(=O)CCCC(=O)OCCCCCCCCCCC)C(C)CCC  
**Mol. weight [g/mol]:** 434.65

## Physical Properties

Property code	Value	Unit	Source
gf	-14.17	kJ/mol	Joback Method
hf	-712.83	kJ/mol	Joback Method
hfus	64.75	kJ/mol	Joback Method
hvap	94.79	kJ/mol	Joback Method
log10ws	-8.37		Crippen Method
logp	7.158		Crippen Method
mvol	393.270	ml/mol	McGowan Method
pc	818.66	kPa	Joback Method
rinpol	2834.00		NIST Webbook
rinpol	2834.00		NIST Webbook
tb	974.42	K	Joback Method
tc	1194.01	K	Joback Method
tf	598.75	K	Joback Method
vc	1.528	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1324.88	J/molxK	974.42	Joback Method
cpg	1344.12	J/molxK	1011.02	Joback Method
cpg	1361.81	J/molxK	1047.62	Joback Method
cpg	1377.99	J/molxK	1084.22	Joback Method
cpg	1392.72	J/molxK	1120.82	Joback Method
cpg	1406.06	J/molxK	1157.41	Joback Method
cpg	1418.06	J/molxK	1194.01	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=U359828&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U359828&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.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>h vap:</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>r in pol:</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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