

# Glutaric acid, hex-4-yn-3-yl octadecyl ester

**Inchi:** InChI=1S/C29H52O4/c1-4-7-8-9-10-11-12-13-14-15-16-17-18-19-20-21-26-32-28(30)24-  
**InchiKey:** XZTFFKSJRJTGTGI-UHFFFAOYSA-N  
**Formula:** C29H52O4  
**SMILES:** CC#CC(CC)OC(=O)CCCC(=O)OCCCCCCCCCCCCCCCCCC  
**Mol. weight [g/mol]:** 464.72

## Physical Properties

Property code	Value	Unit	Source
gf	-74.18	kJ/mol	Joback Method
hf	-864.47	kJ/mol	Joback Method
hfus	76.04	kJ/mol	Joback Method
hvap	100.22	kJ/mol	Joback Method
log10ws	-9.59		Crippen Method
logp	8.306		Crippen Method
mvol	425.750	ml/mol	McGowan Method
pc	714.15	kPa	Joback Method
rinpol	3284.00		NIST Webbook
tb	1024.06	K	Joback Method
tc	1265.38	K	Joback Method
tf	652.01	K	Joback Method
vc	1.663	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1483.40	J/molxK	1024.06	Joback Method
cpg	1504.29	J/molxK	1064.28	Joback Method
cpg	1523.18	J/molxK	1104.50	Joback Method
cpg	1540.16	J/molxK	1144.72	Joback Method
cpg	1555.29	J/molxK	1184.94	Joback Method
cpg	1568.64	J/molxK	1225.16	Joback Method
cpg	1580.29	J/molxK	1265.38	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.cheméo.com/doc/models/crippen_log10ws">https://www.cheméo.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=U359869&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U359869&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>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>m cvol:</b>	McGowan's characteristic volume
<b>pc:</b>	Critical Pressure
<b>r inpol:</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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