

# Glutaric acid, heptadecyl 2-methyloct-5-yn-4-yl ester

Inchi:	InChI=1S/C31H56O4/c1-5-7-9-10-11-12-13-14-15-16-17-18-19-20-21-26-34-30(32)24-22
InchiKey:	LYUYDTPEFZMIGG-UHFFFAOYSA-N
Formula:	C31H56O4
SMILES:	CCC#CC(CC(C)C)OC(=O)CCCC(=O)OCCCCCCCCCCCCCCCCCC
Mol. weight [g/mol]:	492.77

## Physical Properties

Property code	Value	Unit	Source
gf	-59.78	kJ/mol	Joback Method
hf	-911.03	kJ/mol	Joback Method
hfus	77.70	kJ/mol	Joback Method
hvap	104.29	kJ/mol	Joback Method
log10ws	-10.19		Crippen Method
logp	8.943		Crippen Method
mcvol	453.930	ml/mol	McGowan Method
pc	648.78	kPa	Joback Method
rinpol	3913.00		NIST Webbook
rinpol	3913.00		NIST Webbook
tb	1069.38	K	Joback Method
tc	1331.61	K	Joback Method
tf	659.55	K	Joback Method
vc	1.770	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1613.22	J/mol×K	1069.38	Joback Method
cpg	1634.91	J/mol×K	1113.09	Joback Method
cpg	1654.22	J/mol×K	1156.79	Joback Method
cpg	1671.26	J/mol×K	1200.50	Joback Method
cpg	1686.13	J/mol×K	1244.20	Joback Method
cpg	1698.92	J/mol×K	1287.91	Joback Method
cpg	1709.76	J/mol×K	1331.61	Joback Method

# Sources

<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</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=U359614&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U359614&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>mcvol:</b>	McGowan's characteristic volume
<b>pc:</b>	Critical Pressure
<b>rinpola:</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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