

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

<b>Inchi:</b>	InChI=1S/C29H52O4/c1-5-7-9-10-11-12-13-14-15-16-17-18-19-24-32-28(30)22-20-23-29
<b>InchiKey:</b>	JABXUBKZFJBFFS-UHFFFAOYSA-N
<b>Formula:</b>	C29H52O4
<b>SMILES:</b>	CCC#CC(CC(C)C)OC(=O)CCCC(=O)OCCCCCCCCCCCCCCC
<b>Mol. weight [g/mol]:</b>	464.72

## Physical Properties

Property code	Value	Unit	Source
gf	-76.62	kJ/mol	Joback Method
hf	-869.75	kJ/mol	Joback Method
hfus	72.52	kJ/mol	Joback Method
hvap	99.84	kJ/mol	Joback Method
log10ws	-9.35		Crippen Method
logp	8.162		Crippen Method
mcvol	425.750	ml/mol	McGowan Method
pc	717.22	kPa	Joback Method
rinpola	3773.00		NIST Webbook
tb	1023.62	K	Joback Method
tc	1262.95	K	Joback Method
tf	637.01	K	Joback Method
vc	1.657	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1483.65	J/molxK	1023.62	Joback Method
cpg	1504.30	J/molxK	1063.51	Joback Method
cpg	1522.97	J/molxK	1103.40	Joback Method
cpg	1539.74	J/molxK	1143.28	Joback Method
cpg	1554.68	J/molxK	1183.17	Joback Method
cpg	1567.84	J/molxK	1223.06	Joback Method
cpg	1579.32	J/molxK	1262.95	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=U359612&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U359612&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.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.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>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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