

# Glutaric acid, but-3-yn-2-yl oct-3-en-2-yl ester

<b>Inchi:</b>	InChI=1S/C17H26O4/c1-5-7-8-9-11-15(4)21-17(19)13-10-12-16(18)20-14(3)6-2/h2,9,11,
<b>InchiKey:</b>	ZKOPAMBUVNBPHW-PKNBQFBNSA-N
<b>Formula:</b>	C17H26O4
<b>SMILES:</b>	C#CC(C)OC(=O)CCCC(=O)OC(C)C=CCCC
<b>Mol. weight [g/mol]:</b>	294.39

## Physical Properties

Property code	Value	Unit	Source
gf	-77.17	kJ/mol	Joback Method
hf	-485.25	kJ/mol	Joback Method
hfus	41.49	kJ/mol	Joback Method
hvap	70.79	kJ/mol	Joback Method
log10ws	-4.54		Crippen Method
logp	3.400		Crippen Method
mvol	252.370	ml/mol	McGowan Method
pc	1547.57	kPa	Joback Method
rinpol	1868.00		NIST Webbook
rinpol	1868.00		NIST Webbook
tb	734.34	K	Joback Method
tc	925.89	K	Joback Method
tf	437.56	K	Joback Method
vc	0.966	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	716.97	J/molxK	734.34	Joback Method
cpg	732.90	J/molxK	766.26	Joback Method
cpg	747.94	J/molxK	798.19	Joback Method
cpg	762.13	J/molxK	830.11	Joback Method
cpg	775.48	J/molxK	862.04	Joback Method
cpg	788.03	J/molxK	893.96	Joback Method
cpg	799.79	J/molxK	925.89	Joback Method

# Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=U393984&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U393984&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307I">http://pubs.acs.org/doi/abs/10.1021/ci990307I</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>

# 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>hvp:</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>rinp:</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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