

# Glutaric acid, but-3-yn-2-yl 4-methylpent-2-yl ester

<b>Inchi:</b>	InChI=1S/C15H24O4/c1-6-12(4)18-14(16)8-7-9-15(17)19-13(5)10-11(2)3/h1,11-13H,7-10
<b>InchiKey:</b>	WXVNFLDKTMDVDV-UHFFFAOYSA-N
<b>Formula:</b>	C15H24O4
<b>SMILES:</b>	<chem>C#CC(C)OC(=O)CCCC(=O)OC(C)CC(C)C</chem>
<b>Mol. weight [g/mol]:</b>	268.35

## Physical Properties

Property code	Value	Unit	Source
gf	-176.67	kJ/mol	Joback Method
hf	-566.47	kJ/mol	Joback Method
hfus	32.59	kJ/mol	Joback Method
hvap	65.99	kJ/mol	Joback Method
log10ws	-3.60		Crippen Method
logp	2.699		Crippen Method
mcvol	228.490	ml/mol	McGowan Method
pc	1744.82	kPa	Joback Method
rinpola	1617.00		NIST Webbook
tb	683.98	K	Joback Method
tc	874.84	K	Joback Method
tf	405.10	K	Joback Method
vc	0.868	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	630.39	J/molxK	683.98	Joback Method
cpg	646.29	J/molxK	715.79	Joback Method
cpg	661.34	J/molxK	747.60	Joback Method
cpg	675.56	J/molxK	779.41	Joback Method
cpg	688.96	J/molxK	811.22	Joback Method
cpg	701.55	J/molxK	843.03	Joback Method
cpg	713.34	J/molxK	874.84	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=U392483&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U392483&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>

# 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>hvac:</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>mccol:</b>	McGowan's characteristic volume
<b>pc:</b>	Critical Pressure
<b>rinpol:</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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