

# Glutaric acid, but-3-yn-2-yl 2-methylpentyl ester

Inchi:	InChI=1S/C15H24O4/c1-5-8-12(3)11-18-14(16)9-7-10-15(17)19-13(4)6-2/h2,12-13H,5,7-
InchiKey:	ZCNNEJANQNGSDV-UHFFFAOYSA-N
Formula:	C15H24O4
SMILES:	<chem>C#CC(C)OC(=O)CCCC(=O)OCC(C)CCC</chem>
Mol. weight [g/mol]:	268.35

## Physical Properties

Property code	Value	Unit	Source
gf	-174.23	kJ/mol	Joback Method
hf	-561.19	kJ/mol	Joback Method
hfus	36.11	kJ/mol	Joback Method
hvap	66.38	kJ/mol	Joback Method
log10ws	-3.49		Crippen Method
logp	2.701		Crippen Method
mvol	228.490	ml/mol	McGowan Method
pc	1733.22	kPa	Joback Method
rmpol	1707.00		NIST Webbook
tb	684.42	K	Joback Method
tc	872.41	K	Joback Method
tf	420.10	K	Joback Method
vc	0.874	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	629.90	J/mol×K	684.42	Joback Method
cpg	645.54	J/mol×K	715.75	Joback Method
cpg	660.36	J/mol×K	747.08	Joback Method
cpg	674.38	J/mol×K	778.42	Joback Method
cpg	687.61	J/mol×K	809.75	Joback Method
cpg	700.07	J/mol×K	841.08	Joback Method
cpg	711.75	J/mol×K	872.41	Joback Method

# Sources

<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=U391704&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U391704&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>

# 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>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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