

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

Inchi:	InChI=1S/C16H26O4/c1-6-9-14(12(3)4)20-16(18)11-8-10-15(17)19-13(5)7-2/h2,12-14H,6
InchiKey:	JKDKICVZUJIUSK-UHFFFAOYSA-N
Formula:	C16H26O4
SMILES:	<chem>C#CC(C)OC(=O)CCCC(=O)OC(CCC)C(C)C</chem>
Mol. weight [g/mol]:	282.38

## Physical Properties

Property code	Value	Unit	Source
gf	-168.25	kJ/mol	Joback Method
hf	-587.11	kJ/mol	Joback Method
hfus	35.18	kJ/mol	Joback Method
hvap	68.22	kJ/mol	Joback Method
log10ws	-4.02		Crippen Method
logp	3.089		Crippen Method
mcvol	242.580	ml/mol	McGowan Method
pc	1612.88	kPa	Joback Method
rinpola	1710.00		NIST Webbook
rinpola	1710.00		NIST Webbook
tb	706.86	K	Joback Method
tc	896.41	K	Joback Method
tf	416.37	K	Joback Method
vc	0.923	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	685.17	J/molxK	706.86	Joback Method
cpg	701.47	J/molxK	738.45	Joback Method
cpg	716.88	J/molxK	770.04	Joback Method
cpg	731.43	J/molxK	801.63	Joback Method
cpg	745.12	J/molxK	833.22	Joback Method
cpg	757.97	J/molxK	864.82	Joback Method
cpg	769.99	J/molxK	896.41	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=U393727&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U393727&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.cheméo.com/doc/models/crippen_log10ws">https://www.cheméo.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>mcvol:</b>	McGowan's characteristic volume
<b>pc:</b>	Critical Pressure
<b>r in pol:</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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