

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

<b>Inchi:</b>	InChI=1S/C13H20O4/c1-4-6-10-16-12(14)8-7-9-13(15)17-11(3)5-2/h2,11H,4,6-10H2,1,3H
<b>InchiKey:</b>	ASVRPQCLPQTIBM-UHFFFAOYSA-N
<b>Formula:</b>	C13H20O4
<b>SMILES:</b>	C#CC(C)OC(=O)CCCC(=O)OCCCC
<b>Mol. weight [g/mol]:</b>	240.30

## Physical Properties

Property code	Value	Unit	Source
gf	-188.63	kJ/mol	Joback Method
hf	-514.63	kJ/mol	Joback Method
hfus	34.45	kJ/mol	Joback Method
hvap	62.31	kJ/mol	Joback Method
log10ws	-2.90		Crippen Method
logp	2.065		Crippen Method
mcvol	200.310	ml/mol	McGowan Method
pc	2032.72	kPa	Joback Method
rinpola	1616.00		NIST Webbook
rinpola	1616.00		NIST Webbook
tb	639.10	K	Joback Method
tc	827.18	K	Joback Method
tf	412.56	K	Joback Method
vc	0.767	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	523.79	J/molxK	639.10	Joback Method
cpg	538.14	J/molxK	670.45	Joback Method
cpg	551.79	J/molxK	701.79	Joback Method
cpg	564.74	J/molxK	733.14	Joback Method
cpg	577.01	J/molxK	764.49	Joback Method
cpg	588.61	J/molxK	795.84	Joback Method
cpg	599.52	J/molxK	827.18	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=U359874&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U359874&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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