

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

<b>Inchi:</b>	InChI=1S/C17H26O4/c1-4-13(3)20-16(18)11-8-12-17(19)21-15-10-7-6-9-14(15)5-2/h1,13
<b>InchiKey:</b>	INOSLNABDALRAS-UHFFFAOYSA-N
<b>Formula:</b>	C17H26O4
<b>SMILES:</b>	<chem>C#CC(C)OC(=O)CCCC(=O)OC1CCCCC1CC</chem>
<b>Mol. weight [g/mol]:</b>	294.39

## Physical Properties

Property code	Value	Unit	Source
gf	-138.21	kJ/mol	Joback Method
hf	-563.21	kJ/mol	Joback Method
hfus	37.72	kJ/mol	Joback Method
hvap	71.34	kJ/mol	Joback Method
log10ws	-4.34		Crippen Method
logp	3.234		Crippen Method
mvol	245.810	ml/mol	McGowan Method
pc	1693.51	kPa	Joback Method
rinpol	1921.00		NIST Webbook
rinpol	1921.00		NIST Webbook
tb	745.50	K	Joback Method
tc	951.99	K	Joback Method
tf	460.78	K	Joback Method
vc	0.923	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	737.77	J/mol×K	745.50	Joback Method
cpg	756.25	J/mol×K	779.91	Joback Method
cpg	773.51	J/mol×K	814.33	Joback Method
cpg	789.54	J/mol×K	848.74	Joback Method
cpg	804.38	J/mol×K	883.16	Joback Method
cpg	818.03	J/mol×K	917.57	Joback Method
cpg	830.52	J/mol×K	951.99	Joback Method

# Sources

<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>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=U405478&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U405478&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>

# 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>hvpap:</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>rinppl:</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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