

# Glutaric acid, butyl 2,7-dimethyloct-5-yn-7-en-4-yl ester

Inchi:	InChI=1S/C19H30O4/c1-6-7-13-22-18(20)9-8-10-19(21)23-17(14-16(4)5)12-11-15(2)3/h
InchiKey:	DKGGHMLULVYABL-UHFFFAOYSA-N
Formula:	C19H30O4
SMILES:	C=C(C)C#CC(CC(C)C)OC(=O)CCCC(=O)OCCCC
Mol. weight [g/mol]:	322.44

## Physical Properties

Property code	Value	Unit	Source
gf	-81.53	kJ/mol	Joback Method
hf	-547.71	kJ/mol	Joback Method
hfus	44.03	kJ/mol	Joback Method
hvap	76.99	kJ/mol	Joback Method
log10ws	-5.02		Crippen Method
logp	4.037		Crippen Method
mvol	280.550	ml/mol	McGowan Method
pc	1344.71	kPa	Joback Method
rinpol	2083.00		NIST Webbook
rinpol	2083.00		NIST Webbook
tb	791.38	K	Joback Method
tc	987.58	K	Joback Method
tf	508.59	K	Joback Method
vc	1.079	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	834.68	J/mol×K	791.38	Joback Method
cpg	851.65	J/mol×K	824.08	Joback Method
cpg	867.60	J/mol×K	856.78	Joback Method
cpg	882.54	J/mol×K	889.48	Joback Method
cpg	896.48	J/mol×K	922.18	Joback Method
cpg	909.45	J/mol×K	954.88	Joback Method
cpg	921.45	J/mol×K	987.58	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=U359837&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U359837&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>

# 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>hvp:</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>rinp:</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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