

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

Inchi:	InChI=1S/C19H30O4/c1-14(2)10-11-17(12-15(3)4)23-19(21)9-7-8-18(20)22-13-16(5)6/h1
InchiKey:	QSNUCIJDHPHWLB-UHFFFAOYSA-N
Formula:	C19H30O4
SMILES:	<chem>C=C(C)C#CC(CC(C)C)OC(=O)CCCC(=O)OCC(C)C</chem>
Mol. weight [g/mol]:	322.44

## Physical Properties

Property code	Value	Unit	Source
gf	-83.97	kJ/mol	Joback Method
hf	-552.99	kJ/mol	Joback Method
hfus	40.50	kJ/mol	Joback Method
hvap	76.60	kJ/mol	Joback Method
log10ws	-4.78		Crippen Method
logp	3.893		Crippen Method
mcvol	280.550	ml/mol	McGowan Method
pc	1352.64	kPa	Joback Method
rinqol	2042.00		NIST Webbook
tb	790.94	K	Joback Method
tc	989.34	K	Joback Method
tf	493.59	K	Joback Method
vc	1.073	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	835.19	J/molxK	790.94	Joback Method
cpg	852.36	J/molxK	824.01	Joback Method
cpg	868.47	J/molxK	857.07	Joback Method
cpg	883.53	J/molxK	890.14	Joback Method
cpg	897.56	J/molxK	923.21	Joback Method
cpg	910.59	J/molxK	956.27	Joback Method
cpg	922.63	J/molxK	989.34	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=U359836&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U359836&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.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.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>hvac:</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>mccvol:</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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