

# Glutaric acid, isobutyl non-5-yn-3-yl ester

<b>Inchi:</b>	InChI=1S/C18H30O4/c1-5-7-8-9-11-16(6-2)22-18(20)13-10-12-17(19)21-14-15(3)4/h15-1
<b>InchiKey:</b>	IUZKNPXJMWXAY-UHFFFAOYSA-N
<b>Formula:</b>	C18H30O4
<b>SMILES:</b>	CCCC#CCC(CC)OC(=O)CCCC(=O)OCC(C)C
<b>Mol. weight [g/mol]:</b>	310.43

## Physical Properties

Property code	Value	Unit	Source
gf	-169.24	kJ/mol	Joback Method
hf	-642.71	kJ/mol	Joback Method
hfus	44.03	kJ/mol	Joback Method
hvap	75.35	kJ/mol	Joback Method
log10ws	-4.75		Crippen Method
logp	3.871		Crippen Method
mvol	270.760	ml/mol	McGowan Method
pc	1394.37	kPa	Joback Method
rmpol	2074.00		NIST Webbook
tb	771.94	K	Joback Method
tc	964.57	K	Joback Method
tf	513.04	K	Joback Method
vc	1.042	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	802.99	J/mol×K	771.94	Joback Method
cpg	820.04	J/mol×K	804.05	Joback Method
cpg	836.09	J/mol×K	836.15	Joback Method
cpg	851.17	J/mol×K	868.26	Joback Method
cpg	865.27	J/mol×K	900.36	Joback Method
cpg	878.41	J/mol×K	932.47	Joback Method
cpg	890.60	J/mol×K	964.57	Joback Method

# Sources

<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</a>
<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=U359799&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U359799&amp;Units=SI</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>hvap:</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>rinpola:</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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