

# Glutaric acid, 3-methylbut-2-yl non-5-yn-3-yl ester

Inchi:	InChI=1S/C19H32O4/c1-6-8-9-10-12-17(7-2)23-19(21)14-11-13-18(20)22-16(5)15(3)4/h1
InchiKey:	AXDIBNRXVKBTRY-UHFFFAOYSA-N
Formula:	C19H32O4
SMILES:	CCCC#CCC(CC)OC(=O)CCCC(=O)OC(C)C(C)C
Mol. weight [g/mol]:	324.45

## Physical Properties

Property code	Value	Unit	Source
gf	-163.26	kJ/mol	Joback Method
hf	-668.63	kJ/mol	Joback Method
hfus	43.09	kJ/mol	Joback Method
hvap	77.19	kJ/mol	Joback Method
log10ws	-5.28		Crippen Method
logp	4.260		Crippen Method
mvol	284.850	ml/mol	McGowan Method
pc	1307.06	kPa	Joback Method
rinpol	2060.00		NIST Webbook
rinpol	2060.00		NIST Webbook
tb	794.38	K	Joback Method
tc	989.09	K	Joback Method
tf	509.31	K	Joback Method
vc	1.091	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	861.96	J/mol×K	794.38	Joback Method
cpg	879.45	J/mol×K	826.83	Joback Method
cpg	895.88	J/mol×K	859.28	Joback Method
cpg	911.26	J/mol×K	891.74	Joback Method
cpg	925.59	J/mol×K	924.19	Joback Method
cpg	938.89	J/mol×K	956.64	Joback Method
cpg	951.18	J/mol×K	989.09	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=U393951&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U393951&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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