

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

<b>Inchi:</b>	InChI=1S/C17H28O4/c1-4-7-8-9-11-15(6-3)21-17(19)13-10-12-16(18)20-14-5-2/h15H,4-7
<b>InchiKey:</b>	TUXLYNWZTHAAQB-UHFFFAOYSA-N
<b>Formula:</b>	C17H28O4
<b>SMILES:</b>	CCCC#CCC(CC)OC(=O)CCCC(=O)OCCC
<b>Mol. weight [g/mol]:</b>	296.40

## Physical Properties

Property code	Value	Unit	Source
gf	-175.22	kJ/mol	Joback Method
hf	-616.79	kJ/mol	Joback Method
hfus	44.96	kJ/mol	Joback Method
hvap	73.51	kJ/mol	Joback Method
log10ws	-4.57		Crippen Method
logp	3.625		Crippen Method
mcvol	256.670	ml/mol	McGowan Method
pc	1490.74	kPa	Joback Method
rinpola	2021.00		NIST Webbook
tb	749.50	K	Joback Method
tc	940.19	K	Joback Method
tf	516.77	K	Joback Method
vc	0.992	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	744.99	J/molxK	749.50	Joback Method
cpg	761.52	J/molxK	781.28	Joback Method
cpg	777.14	J/molxK	813.06	Joback Method
cpg	791.84	J/molxK	844.85	Joback Method
cpg	805.64	J/molxK	876.63	Joback Method
cpg	818.55	J/molxK	908.41	Joback Method
cpg	830.58	J/molxK	940.19	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=U359798&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U359798&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>mccol:</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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