

# Glutaric acid, hex-4-yn-3-yl 2-methylpent-3-yl ester

Inchi:	InChI=1S/C17H28O4/c1-6-10-14(7-2)20-16(18)11-9-12-17(19)21-15(8-3)13(4)5/h13-15H
InchiKey:	OCECDTNXXDQLCB-UHFFFAOYSA-N
Formula:	C17H28O4
SMILES:	CC#CC(CC)OC(=O)CCCC(=O)OC(CC)C(C)C
Mol. weight [g/mol]:	296.40

## Physical Properties

Property code	Value	Unit	Source
gf	-180.10	kJ/mol	Joback Method
hf	-627.35	kJ/mol	Joback Method
hfus	37.91	kJ/mol	Joback Method
hvap	72.74	kJ/mol	Joback Method
log10ws	-4.44		Crippen Method
logp	3.480		Crippen Method
mvol	256.670	ml/mol	McGowan Method
pc	1509.33	kPa	Joback Method
rinpol	1886.00		NIST Webbook
rinpol	1886.00		NIST Webbook
tb	748.62	K	Joback Method
tc	944.19	K	Joback Method
tf	486.77	K	Joback Method
vc	0.980	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	746.01	J/mol×K	748.62	Joback Method
cpg	762.99	J/mol×K	781.21	Joback Method
cpg	778.98	J/mol×K	813.81	Joback Method
cpg	794.00	J/mol×K	846.40	Joback Method
cpg	808.06	J/mol×K	879.00	Joback Method
cpg	821.15	J/mol×K	911.59	Joback Method
cpg	833.29	J/mol×K	944.19	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=U393496&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U393496&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307I">http://pubs.acs.org/doi/abs/10.1021/ci990307I</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>

# 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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