

# Glutaric acid, hexyl 4-methoxy-2-methylbutyl ester

Inchi:	InChI=1S/C17H32O5/c1-4-5-6-7-12-21-16(18)9-8-10-17(19)22-14-15(2)11-13-20-3/h15H
InchiKey:	LFKYWJGJGVGMMT-UHFFFAOYSA-N
Formula:	C17H32O5
SMILES:	CCCCCOC(=O)CCCC(=O)OCC(C)CCOC
Mol. weight [g/mol]:	316.43

## Physical Properties

Property code	Value	Unit	Source
gf	-483.02	kJ/mol	Joback Method
hf	-1021.31	kJ/mol	Joback Method
hfus	43.02	kJ/mol	Joback Method
hvap	73.77	kJ/mol	Joback Method
log10ws	-3.51		Crippen Method
logp	3.496		Crippen Method
mcvol	271.140	ml/mol	McGowan Method
pc	1306.12	kPa	Joback Method
rinpola	2167.00		NIST Webbook
tb	762.92	K	Joback Method
tc	943.28	K	Joback Method
tf	432.90	K	Joback Method
vc	1.048	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	822.07	J/molxK	762.92	Joback Method
cpg	839.00	J/molxK	792.98	Joback Method
cpg	855.01	J/molxK	823.04	Joback Method
cpg	870.08	J/molxK	853.10	Joback Method
cpg	884.23	J/molxK	883.16	Joback Method
cpg	897.46	J/molxK	913.22	Joback Method
cpg	909.76	J/molxK	943.28	Joback Method
dvisc	0.0009338	Paxs	432.90	Joback Method
dvisc	0.0004495	Paxs	487.90	Joback Method

dvisc	0.0002509	Paxs	542.91	Joback Method
dvisc	0.0001559	Paxs	597.91	Joback Method
dvisc	0.0001050	Paxs	652.91	Joback Method
dvisc	0.0000752	Paxs	707.92	Joback Method
dvisc	0.0000565	Paxs	762.92	Joback Method

## Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=U359415&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U359415&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>
<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>

## Legend

<b>cpg:</b>	Ideal gas heat capacity
<b>dvisc:</b>	Dynamic viscosity
<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>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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