

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

<b>Inchi:</b>	InChI=1S/C17H32O5/c1-14(2)7-6-11-21-16(18)8-5-9-17(19)22-13-15(3)10-12-20-4/h14-1
<b>InchiKey:</b>	AURQYPVLOWIYHQ-UHFFFAOYSA-N
<b>Formula:</b>	C17H32O5
<b>SMILES:</b>	COCCC(C)COC(=O)CCCC(=O)OCCCC(C)C
<b>Mol. weight [g/mol]:</b>	316.43

## Physical Properties

Property code	Value	Unit	Source
gf	-485.46	kJ/mol	Joback Method
hf	-1026.59	kJ/mol	Joback Method
hfus	39.50	kJ/mol	Joback Method
hvap	73.38	kJ/mol	Joback Method
log10ws	-3.27		Crippen Method
logp	3.352		Crippen Method
mcvol	271.140	ml/mol	McGowan Method
pc	1313.70	kPa	Joback Method
rinpola	2130.00		NIST Webbook
tb	762.48	K	Joback Method
tc	944.32	K	Joback Method
tf	417.90	K	Joback Method
vc	1.042	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	822.56	J/molxK	762.48	Joback Method
cpg	839.65	J/molxK	792.79	Joback Method
cpg	855.78	J/molxK	823.09	Joback Method
cpg	870.96	J/molxK	853.40	Joback Method
cpg	885.19	J/molxK	883.71	Joback Method
cpg	898.47	J/molxK	914.02	Joback Method
cpg	910.80	J/molxK	944.32	Joback Method
dvisc	0.0011284	Paxs	417.90	Joback Method
dvisc	0.0004957	Paxs	475.33	Joback Method

dvisc	0.0002600	Paxs	532.76	Joback Method
dvisc	0.0001546	Paxs	590.19	Joback Method
dvisc	0.0001008	Paxs	647.62	Joback Method
dvisc	0.0000705	Paxs	705.05	Joback Method
dvisc	0.0000520	Paxs	762.48	Joback Method

## Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=U359414&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U359414&amp;Units=SI</a>
<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>

## 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>mcvol:</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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