

# Glutaric acid, isobutyl 6-methylhept-2-yl ester

<b>Inchi:</b>	InChI=1S/C17H32O4/c1-13(2)8-6-9-15(5)21-17(19)11-7-10-16(18)20-12-14(3)4/h13-15H
<b>InchiKey:</b>	GQPSNJRMMWVROHU-UHFFFAOYSA-N
<b>Formula:</b>	C17H32O4
<b>SMILES:</b>	CC(C)CCCC(C)OC(=O)CCCC(=O)OCC(C)C
<b>Mol. weight [g/mol]:</b>	300.43

## Physical Properties

Property code	Value	Unit	Source
gf	-382.90	kJ/mol	Joback Method
hf	-899.65	kJ/mol	Joback Method
hfus	34.79	kJ/mol	Joback Method
hvap	70.58	kJ/mol	Joback Method
log10ws	-4.29		Crippen Method
logp	4.114		Crippen Method
mcvol	265.270	ml/mol	McGowan Method
pc	1337.84	kPa	Joback Method
rinpola	1922.00		NIST Webbook
tb	739.62	K	Joback Method
tc	922.00	K	Joback Method
tf	380.67	K	Joback Method
vc	1.018	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	792.48	J/molxK	739.62	Joback Method
cpg	810.02	J/molxK	770.02	Joback Method
cpg	826.62	J/molxK	800.41	Joback Method
cpg	842.29	J/molxK	830.81	Joback Method
cpg	857.04	J/molxK	861.21	Joback Method
cpg	870.89	J/molxK	891.60	Joback Method
cpg	883.84	J/molxK	922.00	Joback Method
dvisc	0.0021500	Paxs	380.67	Joback Method
dvisc	0.0008028	Paxs	440.50	Joback Method

dvisc	0.0003794	Paxs	500.32	Joback Method
dvisc	0.0002104	Paxs	560.14	Joback Method
dvisc	0.0001308	Paxs	619.97	Joback Method
dvisc	0.0000884	Paxs	679.80	Joback Method
dvisc	0.0000636	Paxs	739.62	Joback Method

## Sources

<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>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=U377168&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U377168&amp;Units=SI</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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