

# Glutaric acid, isohexyl 3-oxobut-2-yl ester

<b>Inchi:</b>	InChI=1S/C15H26O5/c1-11(2)7-6-10-19-14(17)8-5-9-15(18)20-13(4)12(3)16/h11,13H,5-
<b>InchiKey:</b>	MCTLURRWPDIDQC-UHFFFAOYSA-N
<b>Formula:</b>	C15H26O5
<b>SMILES:</b>	CC(=O)C(C)OC(=O)CCCC(=O)OCCCC(C)C
<b>Mol. weight [g/mol]:</b>	286.36

## Physical Properties

Property code	Value	Unit	Source
gf	-526.22	kJ/mol	Joback Method
hf	-965.67	kJ/mol	Joback Method
hfus	34.73	kJ/mol	Joback Method
hvap	73.27	kJ/mol	Joback Method
log10ws	-2.98		Crippen Method
logp	2.657		Crippen Method
mcvol	238.660	ml/mol	McGowan Method
pc	1616.77	kPa	Joback Method
rinpol	1933.00		NIST Webbook
rinpol	1933.00		NIST Webbook
tb	748.17	K	Joback Method
tc	936.03	K	Joback Method
tf	423.06	K	Joback Method
vc	0.917	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	700.46	J/molxK	748.17	Joback Method
cpg	715.70	J/molxK	779.48	Joback Method
cpg	730.06	J/molxK	810.79	Joback Method
cpg	743.54	J/molxK	842.10	Joback Method
cpg	756.15	J/molxK	873.41	Joback Method
cpg	767.89	J/molxK	904.72	Joback Method
cpg	778.77	J/molxK	936.03	Joback Method
dvisc	0.0015206	Paxs	423.06	Joback Method

dvisc	0.0007209	Paxs	477.25	Joback Method
dvisc	0.0003979	Paxs	531.43	Joback Method
dvisc	0.0002452	Paxs	585.62	Joback Method
dvisc	0.0001640	Paxs	639.80	Joback Method
dvisc	0.0001168	Paxs	693.98	Joback Method
dvisc	0.0000874	Paxs	748.17	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=U359705&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U359705&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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