

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

<b>Inchi:</b>	InChI=1S/C14H24O5/c1-4-5-6-10-18-13(16)8-7-9-14(17)19-12(3)11(2)15/h12H,4-10H2,1
<b>InchiKey:</b>	KHFSUSIUYPQHJBH-UHFFFAOYSA-N
<b>Formula:</b>	C14H24O5
<b>SMILES:</b>	CCCCCOC(=O)CCCC(=O)OC(C)C(C)=O
<b>Mol. weight [g/mol]:</b>	272.34

## Physical Properties

Property code	Value	Unit	Source
gf	-532.20	kJ/mol	Joback Method
hf	-939.75	kJ/mol	Joback Method
hfus	35.67	kJ/mol	Joback Method
hvap	71.43	kJ/mol	Joback Method
log10ws	-2.80		Crippen Method
logp	2.411		Crippen Method
mvol	224.570	ml/mol	McGowan Method
pc	1737.56	kPa	Joback Method
rinpol	1873.00		NIST Webbook
tb	725.73	K	Joback Method
tc	911.61	K	Joback Method
tf	426.79	K	Joback Method
vc	0.868	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	644.31	J/molxK	725.73	Joback Method
cpg	709.54	J/molxK	880.63	Joback Method
cpg	698.10	J/molxK	849.65	Joback Method
cpg	685.86	J/molxK	818.67	Joback Method
cpg	672.82	J/molxK	787.69	Joback Method
cpg	658.97	J/molxK	756.71	Joback Method
cpg	720.18	J/molxK	911.61	Joback Method
dvisc	0.0001084	Paxs	725.73	Joback Method
dvisc	0.0001419	Paxs	675.91	Joback Method

dvisc	0.0001938	Paxs	626.08	Joback Method
dvisc	0.0002795	Paxs	576.26	Joback Method
dvisc	0.0004318	Paxs	526.44	Joback Method
dvisc	0.0007307	Paxs	476.61	Joback Method
dvisc	0.0013982	Paxs	426.79	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=U359704&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U359704&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>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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