

# Glutaric acid, ethyl 3-methylphenyl ester

<b>Inchi:</b>	InChI=1S/C14H18O4/c1-3-17-13(15)8-5-9-14(16)18-12-7-4-6-11(2)10-12/h4,6-7,10H,3,5
<b>InchiKey:</b>	DCJGDMJDXOWYCY-UHFFFAOYSA-N
<b>Formula:</b>	C14H18O4
<b>SMILES:</b>	CCOC(=O)CCCC(=O)Oc1cccc(C)c1
<b>Mol. weight [g/mol]:</b>	250.29

## Physical Properties

Property code	Value	Unit	Source
gf	-298.06	kJ/mol	Joback Method
hf	-596.83	kJ/mol	Joback Method
hfus	31.24	kJ/mol	Joback Method
hvap	68.01	kJ/mol	Joback Method
log10ws	-3.22		Crippen Method
logp	2.634		Crippen Method
mcvol	199.240	ml/mol	McGowan Method
pc	2155.30	kPa	Joback Method
rinpol	1904.00		NIST Webbook
rinpol	1904.00		NIST Webbook
tb	703.96	K	Joback Method
tc	909.90	K	Joback Method
tf	430.80	K	Joback Method
vc	0.759	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	539.98	J/mol×K	703.96	Joback Method
cpg	603.00	J/mol×K	875.58	Joback Method
cpg	592.16	J/mol×K	841.25	Joback Method
cpg	580.44	J/mol×K	806.93	Joback Method
cpg	567.84	J/mol×K	772.61	Joback Method
cpg	554.36	J/mol×K	738.28	Joback Method
cpg	612.97	J/mol×K	909.90	Joback Method
dvisc	0.0001192	Paxs	703.96	Joback Method

dvisc	0.0001501	Paxs	658.43	Joback Method
dvisc	0.0001956	Paxs	612.91	Joback Method
dvisc	0.0002660	Paxs	567.38	Joback Method
dvisc	0.0003816	Paxs	521.85	Joback Method
dvisc	0.0005866	Paxs	476.33	Joback Method
dvisc	0.0009874	Paxs	430.80	Joback Method

## Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=U358901&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U358901&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>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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