

# Glutaric acid, 3-methylbut-2-yl 2-formylphenyl ester

Inchi:	InChI=1S/C17H22O5/c1-12(2)13(3)21-16(19)9-6-10-17(20)22-15-8-5-4-7-14(15)11-18/h
InchiKey:	KSECMGOHBVOBLT-UHFFFAOYSA-N
Formula:	C17H22O5
SMILES:	CC(C)C(C)OC(=O)CCCC(=O)Oc1ccccc1C=O
Mol. weight [g/mol]:	306.35

## Physical Properties

Property code	Value	Unit	Source
gf	-377.20	kJ/mol	Joback Method
hf	-754.89	kJ/mol	Joback Method
hfus	34.26	kJ/mol	Joback Method
hvap	80.63	kJ/mol	Joback Method
log10ws	-4.11		Crippen Method
logp	3.163		Crippen Method
mcvol	243.080	ml/mol	McGowan Method
pc	1807.70	kPa	Joback Method
rinpol	2254.00		NIST Webbook
rinpol	2254.00		NIST Webbook
tb	820.38	K	Joback Method
tc	1029.72	K	Joback Method
tf	476.61	K	Joback Method
vc	0.932	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	721.60	J/molxK	820.38	Joback Method
cpg	735.50	J/molxK	855.27	Joback Method
cpg	748.32	J/molxK	890.16	Joback Method
cpg	760.06	J/molxK	925.05	Joback Method
cpg	770.73	J/molxK	959.94	Joback Method
cpg	780.36	J/molxK	994.83	Joback Method
cpg	788.96	J/molxK	1029.72	Joback Method
dvisc	0.0009630	Paxs	476.61	Joback Method

dvisc	0.0005014	Paxs	533.90	Joback Method
dvisc	0.0002963	Paxs	591.20	Joback Method
dvisc	0.0001922	Paxs	648.50	Joback Method
dvisc	0.0001337	Paxs	705.79	Joback Method
dvisc	0.0000982	Paxs	763.09	Joback Method
dvisc	0.0000753	Paxs	820.38	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=U390247&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U390247&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>

## 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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