

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

Inchi:	InChI=1S/C19H28O4/c1-15(2)16(3)23-19(21)13-7-12-18(20)22-14-8-11-17-9-5-4-6-10-17
InchiKey:	TZQJVFJSJPXVQFH-UHFFFAOYSA-N
Formula:	C19H28O4
SMILES:	CC(C)C(C)OC(=O)CCCC(=O)OCCc1ccccc1
Mol. weight [g/mol]:	320.42

## Physical Properties

Property code	Value	Unit	Source
gf	-251.21	kJ/mol	Joback Method
hf	-699.12	kJ/mol	Joback Method
hfus	37.53	kJ/mol	Joback Method
hvap	77.70	kJ/mol	Joback Method
log10ws	-4.47		Crippen Method
logp	3.920		Crippen Method
mcvol	269.690	ml/mol	McGowan Method
pc	1475.88	kPa	Joback Method
tb	812.50	K	Joback Method
tc	1015.45	K	Joback Method
tf	444.63	K	Joback Method
vc	1.028	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	820.77	J/molxK	812.50	Joback Method
cpg	837.10	J/molxK	846.32	Joback Method
cpg	852.27	J/molxK	880.15	Joback Method
cpg	866.32	J/molxK	913.97	Joback Method
cpg	879.27	J/molxK	947.80	Joback Method
cpg	891.14	J/molxK	981.62	Joback Method
cpg	901.96	J/molxK	1015.45	Joback Method
dvisc	0.0010535	Paxs	444.63	Joback Method
dvisc	0.0004721	Paxs	505.94	Joback Method
dvisc	0.0002516	Paxs	567.25	Joback Method

dvisc	0.0001517	Paxs	628.57	Joback Method
dvisc	0.0001000	Paxs	689.88	Joback Method
dvisc	0.0000706	Paxs	751.19	Joback Method
dvisc	0.0000525	Paxs	812.50	Joback Method

## Sources

<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=U391771&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U391771&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307l">http://pubs.acs.org/doi/abs/10.1021/ci990307l</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>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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