

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

Inchi:	InChI=1S/C20H30O4/c1-4-18(16(2)3)24-20(22)14-8-13-19(21)23-15-9-12-17-10-6-5-7-1
InchiKey:	ODQMCYJMNDZDQJ-UHFFFAOYSA-N
Formula:	C20H30O4
SMILES:	CCC(OC(=O)CCCC(=O)OCCc1ccccc1)C(C)C
Mol. weight [g/mol]:	334.45

## Physical Properties

Property code	Value	Unit	Source
gf	-242.79	kJ/mol	Joback Method
hf	-719.76	kJ/mol	Joback Method
hfus	40.12	kJ/mol	Joback Method
hvap	79.93	kJ/mol	Joback Method
log10ws	-4.89		Crippen Method
logp	4.311		Crippen Method
mvol	283.780	ml/mol	McGowan Method
pc	1372.76	kPa	Joback Method
rinpol	2359.00		NIST Webbook
rinpol	2359.00		NIST Webbook
tb	835.38	K	Joback Method
tc	1038.17	K	Joback Method
tf	455.90	K	Joback Method
vc	1.083	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	879.37	J/molxK	835.38	Joback Method
cpg	895.86	J/molxK	869.18	Joback Method
cpg	911.16	J/molxK	902.98	Joback Method
cpg	925.30	J/molxK	936.78	Joback Method
cpg	938.31	J/molxK	970.58	Joback Method
cpg	950.22	J/molxK	1004.38	Joback Method
cpg	961.05	J/molxK	1038.17	Joback Method
dvisc	0.0009406	Paxs	455.90	Joback Method

dvisc	0.0004175	Paxs	519.15	Joback Method
dvisc	0.0002211	Paxs	582.39	Joback Method
dvisc	0.0001326	Paxs	645.64	Joback Method
dvisc	0.0000871	Paxs	708.89	Joback Method
dvisc	0.0000613	Paxs	772.13	Joback Method
dvisc	0.0000455	Paxs	835.38	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=U391772&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U391772&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.cheméo.com/doc/models/crippen_log10ws">https://www.cheméo.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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