

# Glutaric acid, 2-methylhex-3-yl 2-methoxybenzyl ester

<b>Inchi:</b>	InChI=1S/C20H30O5/c1-5-9-17(15(2)3)25-20(22)13-8-12-19(21)24-14-16-10-6-7-11-18(
<b>InchiKey:</b>	FGSKXNXMBNAEOH-UHFFFAOYSA-N
<b>Formula:</b>	C20H30O5
<b>SMILES:</b>	CCCC(OC(=O)CCCC(=O)OCc1ccccc1OC)C(C)C
<b>Mol. weight [g/mol]:</b>	350.45

## Physical Properties

Property code	Value	Unit	Source
gf	-357.42	kJ/mol	Joback Method
hf	-863.45	kJ/mol	Joback Method
hfus	40.92	kJ/mol	Joback Method
hvap	83.00	kJ/mol	Joback Method
log10ws	-5.09		Crippen Method
logp	4.277		Crippen Method
mcvol	289.650	ml/mol	McGowan Method
pc	1340.78	kPa	Joback Method
rinpola	2455.00		NIST Webbook
tb	862.78	K	Joback Method
tc	1067.37	K	Joback Method
tf	490.65	K	Joback Method
vc	1.101	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	908.12	J/molxK	862.78	Joback Method
cpg	923.97	J/molxK	896.88	Joback Method
cpg	938.54	J/molxK	930.98	Joback Method
cpg	951.85	J/molxK	965.07	Joback Method
cpg	963.92	J/molxK	999.17	Joback Method
cpg	974.74	J/molxK	1033.27	Joback Method
cpg	984.34	J/molxK	1067.37	Joback Method
dvisc	0.0005303	Paxs	490.65	Joback Method
dvisc	0.0002604	Paxs	552.67	Joback Method

dvisc	0.0001476	Paxs	614.69	Joback Method
dvisc	0.0000928	Paxs	676.72	Joback Method
dvisc	0.0000631	Paxs	738.74	Joback Method
dvisc	0.0000455	Paxs	800.76	Joback Method
dvisc	0.0000344	Paxs	862.78	Joback Method

## Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=U376929&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U376929&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>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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