

# Glutaric acid, 3-methoxybenzyl pentyl ester

<b>Inchi:</b>	InChI=1S/C18H26O5/c1-3-4-5-12-22-17(19)10-7-11-18(20)23-14-15-8-6-9-16(13-15)21-2
<b>InchiKey:</b>	YSZSSJQTCSWGIP-UHFFFAOYSA-N
<b>Formula:</b>	C18H26O5
<b>SMILES:</b>	CCCCCOC(=O)CCCC(=O)OCc1cccc(OC)c1
<b>Mol. weight [g/mol]:</b>	322.40

## Physical Properties

Property code	Value	Unit	Source
gf	-369.38	kJ/mol	Joback Method
hf	-811.61	kJ/mol	Joback Method
hfus	42.79	kJ/mol	Joback Method
hvap	79.32	kJ/mol	Joback Method
log10ws	-4.38		Crippen Method
logp	3.642		Crippen Method
mcvol	261.470	ml/mol	McGowan Method
pc	1531.86	kPa	Joback Method
rinpola	2431.00		NIST Webbook
tb	817.90	K	Joback Method
tc	1017.91	K	Joback Method
tf	498.11	K	Joback Method
vc	1.002	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	790.00	J/molxK	817.90	Joback Method
cpg	805.25	J/molxK	851.23	Joback Method
cpg	819.39	J/molxK	884.57	Joback Method
cpg	832.44	J/molxK	917.90	Joback Method
cpg	844.40	J/molxK	951.24	Joback Method
cpg	855.27	J/molxK	984.57	Joback Method
cpg	865.06	J/molxK	1017.91	Joback Method
dvisc	0.0005083	Paxs	498.11	Joback Method
dvisc	0.0002926	Paxs	551.41	Joback Method

dvisc	0.0001857	Paxs	604.71	Joback Method
dvisc	0.0001268	Paxs	658.00	Joback Method
dvisc	0.0000917	Paxs	711.30	Joback Method
dvisc	0.0000694	Paxs	764.60	Joback Method
dvisc	0.0000544	Paxs	817.90	Joback Method

## Sources

<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>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=U377190&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U377190&amp;Units=SI</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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