

# Glutaric acid, pentyl 1-phenylethyl ester

<b>Inchi:</b>	InChI=1S/C18H26O4/c1-3-4-8-14-21-17(19)12-9-13-18(20)22-15(2)16-10-6-5-7-11-16/h5
<b>InchiKey:</b>	WHHHYXIQWYJVEO-UHFFFAOYSA-N
<b>Formula:</b>	C18H26O4
<b>SMILES:</b>	CCCCCOC(=O)CCCC(=O)OC(C)c1ccccc1
<b>Mol. weight [g/mol]:</b>	306.40

## Physical Properties

Property code	Value	Unit	Source
gf	-257.19	kJ/mol	Joback Method
hf	-673.20	kJ/mol	Joback Method
hfus	38.47	kJ/mol	Joback Method
hvap	75.86	kJ/mol	Joback Method
log10ws	-4.64		Crippen Method
logp	4.194		Crippen Method
mcvol	255.600	ml/mol	McGowan Method
pc	1580.97	kPa	Joback Method
rinqol	2360.00		NIST Webbook
tb	790.06	K	Joback Method
tc	991.28	K	Joback Method
tf	448.36	K	Joback Method
vc	0.978	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	762.47	J/molxK	790.06	Joback Method
cpg	831.62	J/molxK	957.74	Joback Method
cpg	819.87	J/molxK	924.21	Joback Method
cpg	807.11	J/molxK	890.67	Joback Method
cpg	793.30	J/molxK	857.13	Joback Method
cpg	778.43	J/molxK	823.60	Joback Method
cpg	842.38	J/molxK	991.28	Joback Method
dvisc	0.0000657	Paxs	790.06	Joback Method
dvisc	0.0000866	Paxs	733.11	Joback Method

dvisc	0.0001197	Paxs	676.16	Joback Method
dvisc	0.0001755	Paxs	619.21	Joback Method
dvisc	0.0002780	Paxs	562.26	Joback Method
dvisc	0.0004886	Paxs	505.31	Joback Method
dvisc	0.0009909	Paxs	448.36	Joback Method

## Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=U377514&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U377514&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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