

# Glutaric acid, 4-nitrobenzyl pentyl ester

**Inchi:** InChI=1S/C17H23NO6/c1-2-3-4-12-23-16(19)6-5-7-17(20)24-13-14-8-10-15(11-9-14)18(20)  
**InchiKey:** OSYMUBQFZFJXRI-UHFFFAOYSA-N  
**Formula:** C17H23NO6  
**SMILES:** CCCCCOC(=O)CCCC(=O)OCc1ccc([N+](=O)[O-])cc1  
**Mol. weight [g/mol]:** 337.37

## Physical Properties

Property code	Value	Unit	Source
gf	-237.25	kJ/mol	Joback Method
hf	-669.51	kJ/mol	Joback Method
hfus	50.37	kJ/mol	Joback Method
hvap	91.28	kJ/mol	Joback Method
log10ws	-4.91		Crippen Method
logp	3.542		Crippen Method
mcvol	258.930	ml/mol	McGowan Method
pc	1693.51	kPa	Joback Method
rinqol	2644.00		NIST Webbook
tb	924.44	K	Joback Method
tc	1146.52	K	Joback Method
tf	608.22	K	Joback Method
vc	1.010	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	812.38	J/molxK	924.44	Joback Method
cpg	824.62	J/molxK	961.45	Joback Method
cpg	835.65	J/molxK	998.47	Joback Method
cpg	845.49	J/molxK	1035.48	Joback Method
cpg	854.17	J/molxK	1072.49	Joback Method
cpg	861.72	J/molxK	1109.51	Joback Method
cpg	868.15	J/molxK	1146.52	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=U376838&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U376838&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>
<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>

# Legend

<b>cpg:</b>	Ideal gas heat capacity
<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>rinpola:</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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