

# Glutaric acid, di(4-nitrobenzyl) ester

**Inchi:** InChI=1S/C19H18N2O8/c22-18(28-12-14-4-8-16(9-5-14)20(24)25)2-1-3-19(23)29-13-15  
**InchiKey:** FURINKLSDBYAQM-UHFFFAOYSA-N  
**Formula:** C19H18N2O8  
**SMILES:** O=C(CCCC(=O)OCc1ccc([N+](=O)[O-])cc1)OCc1ccc([N+](=O)[O-])cc1  
**Mol. weight [g/mol]:** 402.35

## Physical Properties

Property code	Value	Unit	Source
gf	-82.08	kJ/mol	Joback Method
hf	-496.49	kJ/mol	Joback Method
hfus	60.57	kJ/mol	Joback Method
hvap	115.26	kJ/mol	Joback Method
log10ws	-6.00		Crippen Method
logp	3.460		Crippen Method
mcvol	280.770	ml/mol	McGowan Method
pc	1900.26	kPa	Joback Method
rinpol	3501.00		NIST Webbook
rinpol	3501.00		NIST Webbook
tb	1153.70	K	Joback Method
tc	1420.54	K	Joback Method
tf	813.31	K	Joback Method
vc	1.095	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	893.89	J/mol×K	1153.70	Joback Method
cpg	898.98	J/mol×K	1198.17	Joback Method
cpg	902.59	J/mol×K	1242.65	Joback Method
cpg	904.77	J/mol×K	1287.12	Joback Method
cpg	905.61	J/mol×K	1331.59	Joback Method
cpg	905.17	J/mol×K	1376.07	Joback Method
cpg	903.51	J/mol×K	1420.54	Joback Method

# Sources

<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=U376844&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U376844&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.cheméo.com/doc/models/crippen_log10ws">https://www.cheméo.com/doc/models/crippen_log10ws</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>rinpolar:</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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