

# Glutaric acid, 3-nitrobenzyl nonyl ester

<b>Inchi:</b>	InChI=1S/C21H31NO6/c1-2-3-4-5-6-7-8-15-27-20(23)13-10-14-21(24)28-17-18-11-9-12-
<b>InchiKey:</b>	IHQQLZWLEDALKE-UHFFFAOYSA-N
<b>Formula:</b>	C21H31NO6
<b>SMILES:</b>	CCCCCCCCCOC(=O)CCCC(=O)OCc1cccc([N+](=O)[O-])c1
<b>Mol. weight [g/mol]:</b>	393.47

## Physical Properties

Property code	Value	Unit	Source
gf	-203.57	kJ/mol	Joback Method
hf	-752.07	kJ/mol	Joback Method
hfus	60.73	kJ/mol	Joback Method
hvap	100.18	kJ/mol	Joback Method
log10ws	-6.59		Crippen Method
logp	5.102		Crippen Method
mcvol	315.290	ml/mol	McGowan Method
pc	1262.85	kPa	Joback Method
rinqol	3123.00		NIST Webbook
tb	1015.96	K	Joback Method
tc	1244.92	K	Joback Method
tf	653.30	K	Joback Method
vc	1.234	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1048.19	J/mol×K	1015.96	Joback Method
cpg	1060.90	J/mol×K	1054.12	Joback Method
cpg	1072.19	J/mol×K	1092.28	Joback Method
cpg	1082.12	J/mol×K	1130.44	Joback Method
cpg	1090.71	J/mol×K	1168.60	Joback Method
cpg	1098.02	J/mol×K	1206.76	Joback Method
cpg	1104.09	J/mol×K	1244.92	Joback Method

# Sources

<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=U377467&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U377467&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>

# 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>hvac:</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>mccol:</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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