

# Glutaric acid, 3-nitro-4-methoxybenzyl nonyl ester

Inchi:	InChI=1S/C22H33NO7/c1-3-4-5-6-7-8-9-15-29-21(24)11-10-12-22(25)30-17-18-13-14-20
InchiKey:	VWNDWAXFZBPYQT-UHFFFAOYSA-N
Formula:	C22H33NO7
SMILES:	CCCCCCCCCOC(=O)CCCC(=O)OCc1ccc(OC)c([N+](=O)[O-])c1
Mol. weight [g/mol]:	423.50

## Physical Properties

Property code	Value	Unit	Source
gf	-309.78	kJ/mol	Joback Method
hf	-916.40	kJ/mol	Joback Method
hfus	64.12	kJ/mol	Joback Method
hvap	105.48	kJ/mol	Joback Method
log10ws	-6.71		Crippen Method
logp	5.111		Crippen Method
mcvol	335.250	ml/mol	McGowan Method
pc	1155.35	kPa	Joback Method
rinsol	3251.00		NIST Webbook
tb	1066.24	K	Joback Method
tc	1305.54	K	Joback Method
tf	699.32	K	Joback Method
vc	1.308	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1132.39	J/molxK	1066.24	Joback Method
cpg	1143.74	J/molxK	1106.12	Joback Method
cpg	1153.28	J/molxK	1146.01	Joback Method
cpg	1161.05	J/molxK	1185.89	Joback Method
cpg	1167.06	J/molxK	1225.77	Joback Method
cpg	1171.34	J/molxK	1265.66	Joback Method
cpg	1173.91	J/molxK	1305.54	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=U377047&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U377047&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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