

# Glutaric acid, 3-methyl-2-nitrobenzyl undecyl ester

<b>Inchi:</b>	InChI=1S/C24H37NO6/c1-3-4-5-6-7-8-9-10-11-18-30-22(26)16-13-17-23(27)31-19-21-15
<b>InchiKey:</b>	PNROAMLNEBXVK-UHFFFAOYSA-N
<b>Formula:</b>	C24H37NO6
<b>SMILES:</b>	CCCCCCCCCOC(=O)CCCC(=O)OCc1cccc(C)c1[N+](=O)[O-]
<b>Mol. weight [g/mol]:</b>	435.55

## Physical Properties

Property code	Value	Unit	Source
gf	-187.94	kJ/mol	Joback Method
hf	-825.46	kJ/mol	Joback Method
hfus	68.11	kJ/mol	Joback Method
hvap	107.52	kJ/mol	Joback Method
log10ws	-7.90		Crippen Method
logp	6.191		Crippen Method
mcvol	357.560	ml/mol	McGowan Method
pc	1029.26	kPa	Joback Method
rinqol	3198.00		NIST Webbook
tb	1089.58	K	Joback Method
tc	1335.53	K	Joback Method
tf	699.63	K	Joback Method
vc	1.401	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1228.54	J/molxK	1089.58	Joback Method
cpg	1241.38	J/molxK	1130.57	Joback Method
cpg	1252.49	J/molxK	1171.56	Joback Method
cpg	1261.92	J/molxK	1212.56	Joback Method
cpg	1269.74	J/molxK	1253.55	Joback Method
cpg	1276.00	J/molxK	1294.54	Joback Method
cpg	1280.76	J/molxK	1335.53	Joback Method

# Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=U376741&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U376741&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>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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