

# Glutaric acid, nonyl 2-tert-butyl-6-methylphenyl ester

<b>Inchi:</b>	InChI=1S/C25H40O4/c1-6-7-8-9-10-11-12-19-28-22(26)17-14-18-23(27)29-24-20(2)15-1
<b>InchiKey:</b>	MPVRUUOEVITGGK-UHFFFAOYSA-N
<b>Formula:</b>	C25H40O4
<b>SMILES:</b>	CCCCCCCCCOC(=O)CCCC(=O)Oc1c(C)cccc1C(C)(C)C
<b>Mol. weight [g/mol]:</b>	404.58

## Physical Properties

Property code	Value	Unit	Source
gf	-212.23	kJ/mol	Joback Method
hf	-844.09	kJ/mol	Joback Method
hfus	51.93	kJ/mol	Joback Method
hvap	91.86	kJ/mol	Joback Method
log10ws	-7.46		Crippen Method
logp	6.662		Crippen Method
mvol	354.230	ml/mol	McGowan Method
pc	972.91	kPa	Joback Method
rinpol	2861.00		NIST Webbook
rinpol	2861.00		NIST Webbook
tb	957.39	K	Joback Method
tc	1172.71	K	Joback Method
tf	569.71	K	Joback Method
vc	1.365	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1180.78	J/molxK	957.39	Joback Method
cpg	1197.94	J/molxK	993.28	Joback Method
cpg	1213.73	J/molxK	1029.16	Joback Method
cpg	1228.20	J/molxK	1065.05	Joback Method
cpg	1241.43	J/molxK	1100.93	Joback Method
cpg	1253.45	J/molxK	1136.82	Joback Method
cpg	1264.34	J/molxK	1172.71	Joback Method
dvisc	0.0002619	Paxs	569.71	Joback Method

dvisc	0.0001383	Paxs	634.32	Joback Method
dvisc	0.0000822	Paxs	698.94	Joback Method
dvisc	0.0000533	Paxs	763.55	Joback Method
dvisc	0.0000370	Paxs	828.16	Joback Method
dvisc	0.0000271	Paxs	892.78	Joback Method
dvisc	0.0000207	Paxs	957.39	Joback Method

## Sources

<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>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=U359139&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U359139&amp;Units=SI</a>

## Legend

<b>cpg:</b>	Ideal gas heat capacity
<b>dvisc:</b>	Dynamic viscosity
<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>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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