

# Glutaric acid, 2,3-dimethylphenyl nonyl ester

<b>Inchi:</b>	InChI=1S/C22H34O4/c1-4-5-6-7-8-9-10-17-25-21(23)15-12-16-22(24)26-20-14-11-13-18
<b>InchiKey:</b>	HKEABFLVTOCQTP-UHFFFAOYSA-N
<b>Formula:</b>	C22H34O4
<b>SMILES:</b>	CCCCCCCCCOC(=O)CCCC(=O)Oc1cccc(C)c1C
<b>Mol. weight [g/mol]:</b>	362.50

## Physical Properties

Property code	Value	Unit	Source
gf	-240.33	kJ/mol	Joback Method
hf	-773.42	kJ/mol	Joback Method
hfus	51.57	kJ/mol	Joback Method
hvap	86.48	kJ/mol	Joback Method
log10ws	-6.62		Crippen Method
logp	5.673		Crippen Method
mcvol	311.960	ml/mol	McGowan Method
pc	1159.29	kPa	Joback Method
rinsol	2745.00		NIST Webbook
tb	891.98	K	Joback Method
tc	1096.12	K	Joback Method
tf	533.48	K	Joback Method
vc	1.208	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	996.72	J/molxK	891.98	Joback Method
cpg	1013.19	J/molxK	926.00	Joback Method
cpg	1028.42	J/molxK	960.03	Joback Method
cpg	1042.43	J/molxK	994.05	Joback Method
cpg	1055.25	J/molxK	1028.08	Joback Method
cpg	1066.89	J/molxK	1062.10	Joback Method
cpg	1077.39	J/molxK	1096.12	Joback Method
dvisc	0.0004177	Paxs	533.48	Joback Method
dvisc	0.0002348	Paxs	593.23	Joback Method

dvisc	0.0001467	Paxs	652.98	Joback Method
dvisc	0.0000992	Paxs	712.73	Joback Method
dvisc	0.0000712	Paxs	772.48	Joback Method
dvisc	0.0000537	Paxs	832.23	Joback Method
dvisc	0.0000420	Paxs	891.98	Joback Method

## Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=U359304&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U359304&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>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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