

# Glutaric acid, 2,6-dimethylnon-1-en-3-yn-5-yl nonyl ester

<b>Inchi:</b>	InChI=1S/C25H42O4/c1-6-8-9-10-11-12-13-20-28-24(26)16-14-17-25(27)29-23(19-18-21
<b>InchiKey:</b>	SZWABNDXIVFPMI-UHFFFAOYSA-N
<b>Formula:</b>	C25H42O4
<b>SMILES:</b>	<chem>C=C(C)C#CC(OC(=O)CCCC(=O)OCCCCCCCCC)C(C)CCC</chem>
<b>Mol. weight [g/mol]:</b>	406.60

## Physical Properties

Property code	Value	Unit	Source
gf	-31.01	kJ/mol	Joback Method
hf	-671.55	kJ/mol	Joback Method
hfus	59.57	kJ/mol	Joback Method
hvap	90.34	kJ/mol	Joback Method
log10ws	-7.53		Crippen Method
logp	6.378		Crippen Method
mcvol	365.090	ml/mol	McGowan Method
pc	916.61	kPa	Joback Method
rinsol	2650.00		NIST Webbook
tb	928.66	K	Joback Method
tc	1137.11	K	Joback Method
tf	576.21	K	Joback Method
vc	1.415	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1198.70	J/mol×K	928.66	Joback Method
cpg	1217.25	J/mol×K	963.40	Joback Method
cpg	1234.43	J/mol×K	998.14	Joback Method
cpg	1250.29	J/mol×K	1032.88	Joback Method
cpg	1264.86	J/mol×K	1067.63	Joback Method
cpg	1278.17	J/mol×K	1102.37	Joback Method
cpg	1290.28	J/mol×K	1137.11	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=U359826&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U359826&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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