

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

Inchi:	InChI=1S/C21H34O4/c1-6-8-9-16-24-20(22)12-10-13-21(23)25-19(15-14-17(3)4)18(5)11
InchiKey:	TVMBAHYGEUTBBL-UHFFFAOYSA-N
Formula:	C21H34O4
SMILES:	<chem>C=C(C)C#CC(OC(=O)CCCC(=O)OCCCC)C(C)CCC</chem>
Mol. weight [g/mol]:	350.49

## Physical Properties

Property code	Value	Unit	Source
gf	-64.69	kJ/mol	Joback Method
hf	-588.99	kJ/mol	Joback Method
hfus	49.21	kJ/mol	Joback Method
hvap	81.44	kJ/mol	Joback Method
log10ws	-5.86		Crippen Method
logp	4.818		Crippen Method
mcvol	308.730	ml/mol	McGowan Method
pc	1173.63	kPa	Joback Method
rinpola	2256.00		NIST Webbook
tb	837.14	K	Joback Method
tc	1034.39	K	Joback Method
tf	531.13	K	Joback Method
vc	1.192	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	953.10	J/molxK	837.14	Joback Method
cpg	970.57	J/molxK	870.02	Joback Method
cpg	986.93	J/molxK	902.89	Joback Method
cpg	1002.19	J/molxK	935.77	Joback Method
cpg	1016.39	J/molxK	968.64	Joback Method
cpg	1029.53	J/molxK	1001.52	Joback Method
cpg	1041.66	J/molxK	1034.39	Joback Method

# Sources

<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=U359821&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U359821&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>
<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>

# 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>mccvol:</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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