

# Glutaric acid, nonyl tridec-2-ynyl ester

<b>Inchi:</b>	InChI=1S/C27H48O4/c1-3-5-7-9-11-12-13-14-16-18-20-25-31-27(29)23-21-22-26(28)30-
<b>InchiKey:</b>	SZTSFSXGTQMLAF-UHFFFAOYSA-N
<b>Formula:</b>	C27H48O4
<b>SMILES:</b>	CCCCCCCCC#CCOC(=O)CCCC(=O)OCCCCCCCCC
<b>Mol. weight [g/mol]:</b>	436.67

## Physical Properties

Property code	Value	Unit	Source
gf	-88.58	kJ/mol	Joback Method
hf	-817.91	kJ/mol	Joback Method
hfus	74.38	kJ/mol	Joback Method
hvap	96.16	kJ/mol	Joback Method
log10ws	-8.64		Crippen Method
logp	7.528		Crippen Method
mcvol	397.570	ml/mol	McGowan Method
pc	789.93	kPa	Joback Method
rinpola	3134.00		NIST Webbook
tb	978.74	K	Joback Method
tc	1202.90	K	Joback Method
tf	644.47	K	Joback Method
vc	1.558	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1354.57	J/mol×K	978.74	Joback Method
cpg	1374.64	J/mol×K	1016.10	Joback Method
cpg	1393.03	J/mol×K	1053.46	Joback Method
cpg	1409.79	J/mol×K	1090.82	Joback Method
cpg	1424.97	J/mol×K	1128.18	Joback Method
cpg	1438.62	J/mol×K	1165.54	Joback Method
cpg	1450.80	J/mol×K	1202.90	Joback Method

# Sources

<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>
<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=U360127&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U360127&amp;Units=SI</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>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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