

# Glutaric acid, tridec-2-yn-1-yl dodecyl ester

<b>Inchi:</b>	InChI=1S/C30H54O4/c1-3-5-7-9-11-13-15-17-19-21-23-28-34-30(32)26-24-25-29(31)33-
<b>InchiKey:</b>	TYSZZNBNWDQQUAU-UHFFFAOYSA-N
<b>Formula:</b>	C30H54O4
<b>SMILES:</b>	CCCCCCCCCCC#CCOC(=O)CCCC(=O)OCCCCCCCCCCCCC
<b>Mol. weight [g/mol]:</b>	478.75

## Physical Properties

Property code	Value	Unit	Source
gf	-63.32	kJ/mol	Joback Method
hf	-879.83	kJ/mol	Joback Method
hfus	82.15	kJ/mol	Joback Method
hvap	102.84	kJ/mol	Joback Method
log10ws	-9.90		Crippen Method
logp	8.698		Crippen Method
mvol	439.840	ml/mol	McGowan Method
pc	676.05	kPa	Joback Method
rinpol	3372.00		NIST Webbook
rinpol	3372.00		NIST Webbook
tb	1047.38	K	Joback Method
tc	1302.61	K	Joback Method
tf	678.28	K	Joback Method
vc	1.726	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1547.91	J/mol×K	1047.38	Joback Method
cpg	1569.65	J/mol×K	1089.92	Joback Method
cpg	1589.18	J/mol×K	1132.46	Joback Method
cpg	1606.59	J/mol×K	1175.00	Joback Method
cpg	1621.96	J/mol×K	1217.54	Joback Method
cpg	1635.38	J/mol×K	1260.08	Joback Method
cpg	1646.96	J/mol×K	1302.61	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=U391600&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U391600&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>h vap:</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>rinpolar:</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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