

# Glutaric acid, decyl hex-4-yn-3-yl ester

<b>Inchi:</b>	InChI=1S/C21H36O4/c1-4-7-8-9-10-11-12-13-18-24-20(22)16-14-17-21(23)25-19(6-3)15
<b>InchiKey:</b>	NWTDHQAZOHTYIZ-UHFFFAOYSA-N
<b>Formula:</b>	C21H36O4
<b>SMILES:</b>	CC#CC(CC)OC(=O)CCCC(=O)OCCCCCCCCC
<b>Mol. weight [g/mol]:</b>	352.51

## Physical Properties

Property code	Value	Unit	Source
gf	-141.54	kJ/mol	Joback Method
hf	-699.35	kJ/mol	Joback Method
hfus	55.32	kJ/mol	Joback Method
hvap	82.42	kJ/mol	Joback Method
log10ws	-6.24		Crippen Method
logp	5.186		Crippen Method
mcvol	313.030	ml/mol	McGowan Method
pc	1130.62	kPa	Joback Method
rinqol	2457.00		NIST Webbook
tb	841.02	K	Joback Method
tc	1034.92	K	Joback Method
tf	561.85	K	Joback Method
vc	1.216	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	980.47	J/molxK	841.02	Joback Method
cpg	998.23	J/molxK	873.34	Joback Method
cpg	1014.86	J/molxK	905.65	Joback Method
cpg	1030.39	J/molxK	937.97	Joback Method
cpg	1044.85	J/molxK	970.28	Joback Method
cpg	1058.23	J/molxK	1002.60	Joback Method
cpg	1070.57	J/molxK	1034.92	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=U359861&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U359861&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>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>m cvol:</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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