

# Glutaric acid, di(oct-1-en-3-yl) ester

<b>Inchi:</b>	InChI=1S/C21H36O4/c1-5-9-11-14-18(7-3)24-20(22)16-13-17-21(23)25-19(8-4)15-12-10
<b>InchiKey:</b>	OIKCEYXOKVCELJ-UHFFFAOYSA-N
<b>Formula:</b>	C21H36O4
<b>SMILES:</b>	C=CC(CCCCC)OC(=O)CCCC(=O)OC(C=C)CCCC
<b>Mol. weight [g/mol]:</b>	352.51

## Physical Properties

Property code	Value	Unit	Source
gf	-171.10	kJ/mol	Joback Method
hf	-726.07	kJ/mol	Joback Method
hfus	46.11	kJ/mol	Joback Method
hvap	78.54	kJ/mol	Joback Method
log10ws	-6.27		Crippen Method
logp	5.513		Crippen Method
mcvol	313.030	ml/mol	McGowan Method
pc	1080.64	kPa	Joback Method
rinqol	2176.00		NIST Webbook
tb	824.94	K	Joback Method
tc	1013.79	K	Joback Method
tf	437.23	K	Joback Method
vc	1.210	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	976.43	J/molxK	824.94	Joback Method
cpg	994.15	J/molxK	856.42	Joback Method
cpg	1010.80	J/molxK	887.89	Joback Method
cpg	1026.41	J/molxK	919.37	Joback Method
cpg	1041.00	J/molxK	950.84	Joback Method
cpg	1054.61	J/molxK	982.32	Joback Method
cpg	1067.26	J/molxK	1013.79	Joback Method
dvisc	0.0010788	Paxs	437.23	Joback Method
dvisc	0.0004499	Paxs	501.85	Joback Method

dvisc	0.0002291	Paxs	566.47	Joback Method
dvisc	0.0001339	Paxs	631.09	Joback Method
dvisc	0.0000865	Paxs	695.70	Joback Method
dvisc	0.0000602	Paxs	760.32	Joback Method
dvisc	0.0000443	Paxs	824.94	Joback Method

## Sources

<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=U405360&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U405360&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.cheméo.com/doc/models/crippen_log10ws">https://www.cheméo.com/doc/models/crippen_log10ws</a>

## Legend

<b>cpg:</b>	Ideal gas heat capacity
<b>dvisc:</b>	Dynamic viscosity
<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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