

# Glutaric acid, (2-methylcyclohex-1-enyl)methyl

InChI: InChI= S/C26H42O4/c1-3-4-5-6-7-8-9-10-11-12-15-21-29-25(27)19-16-20-26(28)30-22-2  
tridec-2-yn-1-yl ester

InchiKey: JFQ6JLYZATXKLS-UHFFFAOYSA-N

Formula: C26H42O4

SMILES: CCCCCCCCCC#CCOC(=O)CCCC(=O)OCC1=C(C)CCCC1

Mol. weight [g/mol]: 418.61

## Physical Properties

Property code	Value	Unit	Source
gf	-54.14	kJ/mol	Joback Method
hf	-687.77	kJ/mol	Joback Method
hfus	63.00	kJ/mol	Joback Method
hvap	96.29	kJ/mol	Joback Method
log10ws	-7.97		Crippen Method
logp	6.668		Crippen Method
mvol	368.320	ml/mol	McGowan Method
pc	965.67	kPa	Joback Method
rinpol	3054.00		NIST Webbook
rinpol	3054.00		NIST Webbook
tb	989.20	K	Joback Method
tc	1211.14	K	Joback Method
tf	670.62	K	Joback Method
vc	1.421	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1250.36	J/molxK	989.20	Joback Method
cpg	1267.88	J/molxK	1026.19	Joback Method
cpg	1283.79	J/molxK	1063.18	Joback Method
cpg	1298.11	J/molxK	1100.17	Joback Method
cpg	1310.91	J/molxK	1137.16	Joback Method
cpg	1322.21	J/molxK	1174.15	Joback Method
cpg	1332.06	J/molxK	1211.14	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=U405511&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U405511&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>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>rinpola:</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

Latest version available from:

<https://www.cheméo.com/cid/86-617-2/Glutaric-acid-2-methylcyclohex-1-enyl-methyl-tridec-2-yn-1-yl-ester.pdf>

Generated by Cheméo on 2024-04-26 09:34:16.934403504 +0000 UTC m=+16413305.854980820.

Cheméo (<https://www.cheméo.com>) is the biggest free database of chemical and physical data for the process industry.