

# Glutaric acid, di(non-5-yn-3-yl) ester

**Inchi:** InChI=1S/C23H36O4/c1-5-9-11-13-16-20(7-3)26-22(24)18-15-19-23(25)27-21(8-4)17-14  
**InchiKey:** RINRYEIEVQJOER-UHFFFAOYSA-N  
**Formula:** C23H36O4  
**SMILES:** CCCC#CCC(CC)OC(=O)CCCC(=O)OC(CC)CC#CCCC  
**Mol. weight [g/mol]:** 376.53

## Physical Properties

Property code	Value	Unit	Source
gf	75.66	kJ/mol	Joback Method
hf	-473.61	kJ/mol	Joback Method
hfus	60.10	kJ/mol	Joback Method
hvap	88.63	kJ/mol	Joback Method
log10ws	-6.99		Crippen Method
logp	5.188		Crippen Method
mvol	332.610	ml/mol	McGowan Method
pc	1112.59	kPa	Joback Method
rinpol	2542.00		NIST Webbook
rinpol	2542.00		NIST Webbook
tb	895.34	K	Joback Method
tc	1102.35	K	Joback Method
tf	675.49	K	Joback Method
vc	1.284	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1050.74	J/mol×K	895.34	Joback Method
cpg	1068.20	J/mol×K	929.84	Joback Method
cpg	1084.38	J/mol×K	964.34	Joback Method
cpg	1099.31	J/mol×K	998.85	Joback Method
cpg	1113.02	J/mol×K	1033.35	Joback Method
cpg	1125.52	J/mol×K	1067.85	Joback Method
cpg	1136.85	J/mol×K	1102.35	Joback Method

# Sources

<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=U359816&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U359816&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>

# 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>hvp:</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>rinp:</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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