

# Glutaric acid, 3-methylbutyl tridec-2-yn-1-yl ester

Inchi:	InChI=1S/C23H40O4/c1-4-5-6-7-8-9-10-11-12-13-14-19-26-22(24)16-15-17-23(25)27-20
InchiKey:	JANKHBOOFSPMDY-UHFFFAOYSA-N
Formula:	C23H40O4
SMILES:	CCCCCCCCC#CCOC(=O)CCCC(=O)OCCC(C)C
Mol. weight [g/mol]:	380.56

## Physical Properties

Property code	Value	Unit	Source
gf	-124.70	kJ/mol	Joback Method
hf	-740.63	kJ/mol	Joback Method
hfus	60.50	kJ/mol	Joback Method
hvap	86.87	kJ/mol	Joback Method
log10ws	-6.73		Crippen Method
logp	5.823		Crippen Method
mvol	341.210	ml/mol	McGowan Method
pc	997.65	kPa	Joback Method
rinpol	2653.00		NIST Webbook
rinpol	2653.00		NIST Webbook
tb	886.78	K	Joback Method
tc	1086.62	K	Joback Method
tf	584.39	K	Joback Method
vc	1.327	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1102.99	J/molxK	886.78	Joback Method
cpg	1121.36	J/molxK	920.09	Joback Method
cpg	1138.48	J/molxK	953.39	Joback Method
cpg	1154.37	J/molxK	986.70	Joback Method
cpg	1169.05	J/molxK	1020.00	Joback Method
cpg	1182.55	J/molxK	1053.31	Joback Method
cpg	1194.89	J/molxK	1086.62	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=U393310&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U393310&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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