

# Glutaric acid, butyl tridec-2-ynyl ester

<b>Inchi:</b>	InChI=1S/C22H38O4/c1-3-5-7-8-9-10-11-12-13-14-15-20-26-22(24)18-16-17-21(23)25-1
<b>InchiKey:</b>	HTUSNTDCBHOVKU-UHFFFAOYSA-N
<b>Formula:</b>	C22H38O4
<b>SMILES:</b>	CCCCCCCCC#CCOC(=O)CCCC(=O)OCCCC
<b>Mol. weight [g/mol]:</b>	366.53

## Physical Properties

Property code	Value	Unit	Source
gf	-130.68	kJ/mol	Joback Method
hf	-714.71	kJ/mol	Joback Method
hfus	61.43	kJ/mol	Joback Method
hvap	85.03	kJ/mol	Joback Method
log10ws	-6.55		Crippen Method
logp	5.577		Crippen Method
mvol	327.120	ml/mol	McGowan Method
pc	1055.51	kPa	Joback Method
rpol	2630.00		NIST Webbook
tb	864.34	K	Joback Method
tc	1060.10	K	Joback Method
tf	588.12	K	Joback Method
vc	1.278	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1040.92	J/mol×K	864.34	Joback Method
cpg	1058.93	J/mol×K	896.97	Joback Method
cpg	1075.77	J/mol×K	929.59	Joback Method
cpg	1091.47	J/mol×K	962.22	Joback Method
cpg	1106.04	J/mol×K	994.85	Joback Method
cpg	1119.52	J/mol×K	1027.47	Joback Method
cpg	1131.91	J/mol×K	1060.10	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=U360122&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U360122&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307I">http://pubs.acs.org/doi/abs/10.1021/ci990307I</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

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