

# Glutaric acid, but-3-yn-2-yl 2,6-dimethylnon-1-en-3-yn-5-yl ester

**Inchi:** InChI=1S/C20H28O4/c1-7-10-16(5)18(14-13-15(3)4)24-20(22)12-9-11-19(21)23-17(6)8-2

**InchiKey:** QKHWMNGXRWZDU-UHFFFAOYSA-N

**Formula:** C20H28O4

**SMILES:** C#CC(C)OC(=O)CCCC(=O)OC(C#CC(=C)C)C(C)CCC

**Mol. weight [g/mol]:** 332.43

## Physical Properties

Property code	Value	Unit	Source
gf	147.52	kJ/mol	Joback Method
hf	-281.73	kJ/mol	Joback Method
hfus	46.07	kJ/mol	Joback Method
hvap	78.68	kJ/mol	Joback Method
log10ws	-5.34		Crippen Method
logp	3.649		Crippen Method
mcvol	286.040	ml/mol	McGowan Method
pc	1405.90	kPa	Joback Method
rinpol	2015.00		NIST Webbook
rinpol	2015.00		NIST Webbook
tb	803.94	K	Joback Method
tc	1008.84	K	Joback Method
tf	551.83	K	Joback Method
vc	1.091	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	839.02	J/mol×K	803.94	Joback Method
cpg	855.60	J/mol×K	838.09	Joback Method
cpg	871.12	J/mol×K	872.24	Joback Method
cpg	885.61	J/mol×K	906.39	Joback Method
cpg	899.08	J/mol×K	940.54	Joback Method
cpg	911.57	J/mol×K	974.69	Joback Method
cpg	923.11	J/mol×K	1008.84	Joback Method

# Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=U393962&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U393962&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</a>
<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>

# 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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