

# Glutaric acid, but-3-yl-2-yn 1-naphthyl ester

**Inchi:** InChI=1S/C19H18O4/c1-3-14(2)22-18(20)12-7-13-19(21)23-17-11-6-9-15-8-4-5-10-16(15)  
**InchiKey:** NOCVIMGDWCKNBF-UHFFFAOYSA-N  
**Formula:** C19H18O4  
**SMILES:** C#CC(C)OC(=O)CCCC(=O)Oc1cccc2ccccc12  
**Mol. weight [g/mol]:** 310.34

## Physical Properties

Property code	Value	Unit	Source
gf	71.32	kJ/mol	Joback Method
hf	-222.34	kJ/mol	Joback Method
hfus	40.66	kJ/mol	Joback Method
hvap	80.25	kJ/mol	Joback Method
log10ws	-5.29		Crippen Method
logp	3.480		Crippen Method
mcvol	241.630	ml/mol	McGowan Method
pc	2005.50	kPa	Joback Method
rinpola	2469.00		NIST Webbook
rinpola	2469.00		NIST Webbook
tb	827.02	K	Joback Method
tc	1054.67	K	Joback Method
tf	551.82	K	Joback Method
vc	0.917	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	691.19	J/molxK	827.02	Joback Method
cpg	704.79	J/molxK	864.96	Joback Method
cpg	717.35	J/molxK	902.90	Joback Method
cpg	728.91	J/molxK	940.84	Joback Method
cpg	739.54	J/molxK	978.78	Joback Method
cpg	749.30	J/molxK	1016.72	Joback Method
cpg	758.26	J/molxK	1054.67	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=U393328&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U393328&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>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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