

# 4-Oxo-4-phenylbutyric acid, 2-methyloct-5-yn-4-yl ester

**Inchi:** InChI=1S/C19H24O3/c1-4-5-11-17(14-15(2)3)22-19(21)13-12-18(20)16-9-7-6-8-10-16/h6  
**InchiKey:** KDIQZXWQIFWWPS-UHFFFAOYSA-N  
**Formula:** C19H24O3  
**SMILES:** CCC#CC(CC(C)C)OC(=O)CCC(=O)c1ccccc1  
**Mol. weight [g/mol]:** 300.39

## Physical Properties

Property code	Value	Unit	Source
gf	56.59	kJ/mol	Joback Method
hf	-294.60	kJ/mol	Joback Method
hfus	39.47	kJ/mol	Joback Method
hvap	77.44	kJ/mol	Joback Method
log10ws	-5.26		Crippen Method
logp	4.021		Crippen Method
mcvol	255.220	ml/mol	McGowan Method
pc	1699.10	kPa	Joback Method
tb	799.08	K	Joback Method
tc	1018.57	K	Joback Method
tf	528.50	K	Joback Method
vc	0.972	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	742.01	J/molxK	799.08	Joback Method
cpg	758.31	J/molxK	835.66	Joback Method
cpg	773.42	J/molxK	872.24	Joback Method
cpg	787.39	J/molxK	908.82	Joback Method
cpg	800.26	J/molxK	945.40	Joback Method
cpg	812.08	J/molxK	981.99	Joback Method
cpg	822.88	J/molxK	1018.57	Joback Method

# Sources

<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=U406983&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U406983&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>
<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>

# 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>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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