

# Butyric acid, 2-phenyl-, 2-methyloct-5-yn-4-yl ester

Inchi:	InChI=1S/C19H26O2/c1-5-7-13-17(14-15(3)4)21-19(20)18(6-2)16-11-9-8-10-12-16/h8-12
InchiKey:	LOJIOLGLNIGEJX-UHFFFAOYSA-N
Formula:	C19H26O2
SMILES:	CCC#CC(CC(C)C)OC(=O)C(CC)c1ccccc1
Mol. weight [g/mol]:	286.41

## Physical Properties

Property code	Value	Unit	Source
gf	183.07	kJ/mol	Joback Method
hf	-187.30	kJ/mol	Joback Method
hfus	34.35	kJ/mol	Joback Method
hvap	70.31	kJ/mol	Joback Method
log10ws	-5.37		Crippen Method
logp	4.552		Crippen Method
mvol	253.650	ml/mol	McGowan Method
pc	1624.60	kPa	Joback Method
rinpol	1853.00		NIST Webbook
tb	744.77	K	Joback Method
tc	961.83	K	Joback Method
tf	463.57	K	Joback Method
vc	0.960	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	723.15	J/mol×K	744.77	Joback Method
cpg	741.64	J/mol×K	780.95	Joback Method
cpg	758.91	J/mol×K	817.12	Joback Method
cpg	775.00	J/mol×K	853.30	Joback Method
cpg	789.95	J/mol×K	889.47	Joback Method
cpg	803.81	J/mol×K	925.65	Joback Method
cpg	816.62	J/mol×K	961.83	Joback Method

# Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=U406918&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U406918&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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