

# 4-Butylbenzoic acid, but-3-yn-2-yl ester

<b>Inchi:</b>	InChI=1S/C15H18O2/c1-4-6-7-13-8-10-14(11-9-13)15(16)17-12(3)5-2/h2,8-12H,4,6-7H2
<b>InchiKey:</b>	WDPXNICGYXUUQU-UHFFFAOYSA-N
<b>Formula:</b>	C15H18O2
<b>SMILES:</b>	<chem>C#CC(C)OC(=O)c1ccc(CCCC)cc1</chem>
<b>Mol. weight [g/mol]:</b>	230.30

## Physical Properties

Property code	Value	Unit	Source
gf	164.91	kJ/mol	Joback Method
hf	-86.05	kJ/mol	Joback Method
hfus	30.50	kJ/mol	Joback Method
hvap	60.55	kJ/mol	Joback Method
log10ws	-4.52		Crippen Method
logp	3.208		Crippen Method
mvol	197.290	ml/mol	McGowan Method
pc	2183.60	kPa	Joback Method
rinpol	1715.00		NIST Webbook
rinpol	1715.00		NIST Webbook
tb	640.23	K	Joback Method
tc	854.72	K	Joback Method
tf	401.88	K	Joback Method
vc	0.748	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	501.55	J/mol×K	640.23	Joback Method
cpg	517.49	J/mol×K	675.98	Joback Method
cpg	532.47	J/mol×K	711.73	Joback Method
cpg	546.52	J/mol×K	747.48	Joback Method
cpg	559.66	J/mol×K	783.22	Joback Method
cpg	571.94	J/mol×K	818.97	Joback Method
cpg	583.38	J/mol×K	854.72	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=U292519&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U292519&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307l">http://pubs.acs.org/doi/abs/10.1021/ci990307l</a>
<b>Crippen Method:</b>	<a href="https://www.cheméo.com/doc/models/crippen_log10ws">https://www.cheméo.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>h vap:</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>r in pol:</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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