

# 4-Butylbenzoic acid, tridec-2-ynyl ester

<b>Inchi:</b>	InChI=1S/C24H36O2/c1-3-5-7-8-9-10-11-12-13-14-15-21-26-24(25)23-19-17-22(18-20-2
<b>InchiKey:</b>	FNYBMLUZFCIXFZ-UHFFFAOYSA-N
<b>Formula:</b>	C24H36O2
<b>SMILES:</b>	CCCCCCCCC#CCOC(=O)c1ccc(CCCC)cc1
<b>Mol. weight [g/mol]:</b>	356.54

## Physical Properties

Property code	Value	Unit	Source
gf	222.86	kJ/mol	Joback Method
hf	-286.13	kJ/mol	Joback Method
hfus	57.48	kJ/mol	Joback Method
hvap	83.26	kJ/mol	Joback Method
log10ws	-8.17		Crippen Method
logp	6.720		Crippen Method
mcvol	324.100	ml/mol	McGowan Method
pc	1111.11	kPa	Joback Method
rinpol	2685.40		NIST Webbook
tb	865.47	K	Joback Method
tc	1069.81	K	Joback Method
tf	577.44	K	Joback Method
vc	1.258	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1016.28	J/molxK	865.47	Joback Method
cpg	1034.71	J/molxK	899.53	Joback Method
cpg	1051.95	J/molxK	933.58	Joback Method
cpg	1068.06	J/molxK	967.64	Joback Method
cpg	1083.07	J/molxK	1001.70	Joback Method
cpg	1097.03	J/molxK	1035.76	Joback Method
cpg	1109.98	J/molxK	1069.81	Joback Method

# Sources

<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=U292528&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U292528&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.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</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>hvac:</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>mccol:</b>	McGowan's characteristic volume
<b>pc:</b>	Critical Pressure
<b>rinpol:</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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