

# 4-Butylbenzoic acid, undec-2-enyl ester

<b>Inchi:</b>	InChI=1S/C22H34O2/c1-3-5-7-8-9-10-11-12-13-19-24-22(23)21-17-15-20(16-18-21)14-6
<b>InchiKey:</b>	HQPQCTLGQQAYAS-OUKQBFOZSA-N
<b>Formula:</b>	C22H34O2
<b>SMILES:</b>	CCCCCCCCC=CCOC(=O)c1ccc(CCCC)cc1
<b>Mol. weight [g/mol]:</b>	330.50

## Physical Properties

Property code	Value	Unit	Source
gf	83.44	kJ/mol	Joback Method
hf	-399.93	kJ/mol	Joback Method
hfus	49.38	kJ/mol	Joback Method
hvap	76.62	kJ/mol	Joback Method
log10ws	-7.39		Crippen Method
logp	6.493		Crippen Method
mcvol	300.220	ml/mol	McGowan Method
pc	1176.05	kPa	Joback Method
rinpol	2504.50		NIST Webbook
rinpol	2504.50		NIST Webbook
tb	814.87	K	Joback Method
tc	1011.12	K	Joback Method
tf	443.72	K	Joback Method
vc	1.163	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	919.79	J/molxK	814.87	Joback Method
cpg	938.00	J/molxK	847.58	Joback Method
cpg	955.15	J/molxK	880.29	Joback Method
cpg	971.29	J/molxK	913.00	Joback Method
cpg	986.48	J/molxK	945.70	Joback Method
cpg	1000.75	J/molxK	978.41	Joback Method
cpg	1014.17	J/molxK	1011.12	Joback Method
dvisc	0.0008023	Paxs	443.72	Joback Method

dvisc	0.0003802	Paxs	505.58	Joback Method
dvisc	0.0002120	Paxs	567.44	Joback Method
dvisc	0.0001326	Paxs	629.30	Joback Method
dvisc	0.0000902	Paxs	691.15	Joback Method
dvisc	0.0000654	Paxs	753.01	Joback Method
dvisc	0.0000498	Paxs	814.87	Joback Method

## Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=U292527&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U292527&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>dvisc:</b>	Dynamic viscosity
<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>mccvol:</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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