

# 4-Butylbenzoic acid, heptyl ester

<b>Inchi:</b>	InChI=1S/C18H28O2/c1-3-5-7-8-9-15-20-18(19)17-13-11-16(12-14-17)10-6-4-2/h11-14H
<b>InchiKey:</b>	NJLHIWNIWNPENN-UHFFFAOYSA-N
<b>Formula:</b>	C18H28O2
<b>SMILES:</b>	CCCCCCCOC(=O)c1ccc(CCCC)cc1
<b>Mol. weight [g/mol]:</b>	276.41

## Physical Properties

Property code	Value	Unit	Source
gf	-30.46	kJ/mol	Joback Method
hf	-434.59	kJ/mol	Joback Method
hfus	38.81	kJ/mol	Joback Method
hvap	67.76	kJ/mol	Joback Method
log10ws	-5.87		Crippen Method
logp	5.156		Crippen Method
mcvol	248.160	ml/mol	McGowan Method
pc	1497.67	kPa	Joback Method
rinpol	2118.00		NIST Webbook
tb	719.19	K	Joback Method
tc	912.00	K	Joback Method
tf	403.72	K	Joback Method
vc	0.960	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	710.68	J/molxK	719.19	Joback Method
cpg	789.43	J/molxK	879.87	Joback Method
cpg	775.53	J/molxK	847.73	Joback Method
cpg	760.73	J/molxK	815.60	Joback Method
cpg	745.01	J/molxK	783.46	Joback Method
cpg	728.33	J/molxK	751.33	Joback Method
cpg	802.46	J/molxK	912.00	Joback Method
dvisc	0.0000958	Paxs	719.19	Joback Method
dvisc	0.0001240	Paxs	666.61	Joback Method

dvisc	0.0001678	Paxs	614.03	Joback Method
dvisc	0.0002404	Paxs	561.46	Joback Method
dvisc	0.0003708	Paxs	508.88	Joback Method
dvisc	0.0006322	Paxs	456.30	Joback Method
dvisc	0.0012384	Paxs	403.72	Joback Method

## Sources

<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>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=U292322&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U292322&amp;Units=SI</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>mcvol:</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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