

# Hexyl p-butoxybenzoate

<b>Inchi:</b>	InChI=1S/C17H26O3/c1-3-5-7-8-14-20-17(18)15-9-11-16(12-10-15)19-13-6-4-2/h9-12H,3
<b>InchiKey:</b>	JFMJCSJDUYHPOI-UHFFFAOYSA-N
<b>Formula:</b>	C17H26O3
<b>SMILES:</b>	CCCCCOC(=O)c1ccc(OCCCC)cc1
<b>Mol. weight [g/mol]:</b>	278.39

## Physical Properties

Property code	Value	Unit	Source
gf	-143.88	kJ/mol	Joback Method
hf	-546.17	kJ/mol	Joback Method
hfus	37.41	kJ/mol	Joback Method
hvap	67.94	kJ/mol	Joback Method
log10ws	-5.18		Crippen Method
logp	4.603		Crippen Method
mvol	239.940	ml/mol	McGowan Method
pc	1593.62	kPa	Joback Method
rinpol	2346.00		NIST Webbook
rinpol	2358.00		NIST Webbook
rinpol	2336.00		NIST Webbook
rinpol	2333.00		NIST Webbook
tb	718.73	K	Joback Method
tc	912.24	K	Joback Method
tf	414.68	K	Joback Method
vc	0.921	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	683.80	J/molxK	718.73	Joback Method
cpg	700.78	J/molxK	750.98	Joback Method
cpg	716.81	J/molxK	783.23	Joback Method
cpg	731.90	J/molxK	815.49	Joback Method
cpg	746.06	J/molxK	847.74	Joback Method
cpg	759.31	J/molxK	879.99	Joback Method

cpg	771.65	J/molxK	912.24	Joback Method
dvisc	0.0009484	Paxs	414.68	Joback Method
dvisc	0.0005072	Paxs	465.36	Joback Method
dvisc	0.0003067	Paxs	516.03	Joback Method
dvisc	0.0002029	Paxs	566.71	Joback Method
dvisc	0.0001437	Paxs	617.38	Joback Method
dvisc	0.0001072	Paxs	668.06	Joback Method
dvisc	0.0000834	Paxs	718.73	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=R578866&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R578866&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>

## 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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