

# Hexyl p-butylaminobenzoate

<b>Inchi:</b>	InChI=1S/C17H27NO2/c1-3-5-7-8-14-20-17(19)15-9-11-16(12-10-15)18-13-6-4-2/h9-12,17,20
<b>InchiKey:</b>	FWMKKWXXSYIKQG-UHFFFAOYSA-N
<b>Formula:</b>	C17H27NO2
<b>SMILES:</b>	CCCCCOC(=O)c1ccc(NCCCC)cc1
<b>Mol. weight [g/mol]:</b>	277.40

## Physical Properties

Property code	Value	Unit	Source
gf	50.51	kJ/mol	Joback Method
hf	-360.48	kJ/mol	Joback Method
hfus	41.32	kJ/mol	Joback Method
hvap	71.97	kJ/mol	Joback Method
log10ws	-5.07		Crippen Method
logp	4.636		Crippen Method
mcvol	244.050	ml/mol	McGowan Method
pc	1632.49	kPa	Joback Method
rinpol	2545.00		NIST Webbook
rinpol	2575.00		NIST Webbook
rinpol	2558.00		NIST Webbook
tb	746.48	K	Joback Method
tc	942.49	K	Joback Method
tf	445.11	K	Joback Method
vc	0.939	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	714.05	J/molxK	746.48	Joback Method
cpg	730.74	J/molxK	779.15	Joback Method
cpg	746.44	J/molxK	811.82	Joback Method
cpg	761.19	J/molxK	844.48	Joback Method
cpg	775.02	J/molxK	877.15	Joback Method
cpg	787.94	J/molxK	909.82	Joback Method
cpg	800.00	J/molxK	942.49	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=R578871&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R578871&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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