

# 4-n-Butylphenol, pentafluorobenzoyl ester

<b>Inchi:</b>	InChI=1S/C17H13F5O2/c1-2-3-4-9-5-7-10(8-6-9)24-17(23)11-12(18)14(20)16(22)15(21)
<b>InchiKey:</b>	JMRWZAYNBMAKLD-UHFFFAOYSA-N
<b>Formula:</b>	C17H13F5O2
<b>SMILES:</b>	CCCCc1ccc(OC(=O)c2c(F)c(F)c(F)c(F)c2F)cc1
<b>Mol. weight [g/mol]:</b>	344.28

## Physical Properties

Property code	Value	Unit	Source
gf	-948.67	kJ/mol	Joback Method
hf	-1215.32	kJ/mol	Joback Method
hfus	43.72	kJ/mol	Joback Method
hvap	67.03	kJ/mol	Joback Method
log10ws	-6.86		Crippen Method
logp	4.944		Crippen Method
mcvol	219.160	ml/mol	McGowan Method
pc	1656.49	kPa	Joback Method
rinpol	1872.90		NIST Webbook
rinpol	1879.30		NIST Webbook
rinpol	1875.90		NIST Webbook
rinpol	1872.90		NIST Webbook
tb	744.24	K	Joback Method
tc	938.48	K	Joback Method
tf	484.42	K	Joback Method
vc	0.885	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	605.46	J/molxK	744.24	Joback Method
cpg	618.07	J/molxK	776.61	Joback Method
cpg	629.89	J/molxK	808.99	Joback Method
cpg	640.91	J/molxK	841.36	Joback Method
cpg	651.16	J/molxK	873.73	Joback Method
cpg	660.65	J/molxK	906.11	Joback Method

## Sources

<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307I">http://pubs.acs.org/doi/abs/10.1021/ci990307I</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=R434454&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R434454&amp;Units=SI</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>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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