

# Benzoic acid, 4-(propylamino)-, methyl ester

<b>Inchi:</b>	InChI=1S/C11H15NO2/c1-3-8-12-10-6-4-9(5-7-10)11(13)14-2/h4-7,12H,3,8H2,1-2H3
<b>InchiKey:</b>	NHSSHRRBSAYAPE-UHFFFAOYSA-N
<b>Formula:</b>	C11H15NO2
<b>SMILES:</b>	CCCNc1ccc(C(=O)OC)cc1
<b>Mol. weight [g/mol]:</b>	193.24

## Physical Properties

Property code	Value	Unit	Source
gf	-0.01	kJ/mol	Joback Method
hf	-236.64	kJ/mol	Joback Method
hfus	25.78	kJ/mol	Joback Method
hvap	58.61	kJ/mol	Joback Method
log10ws	-2.56		Crippen Method
logp	2.295		Crippen Method
mcvol	159.510	ml/mol	McGowan Method
pc	2773.00	kPa	Joback Method
rinpol	1778.00		NIST Webbook
rinpol	1778.00		NIST Webbook
tb	609.20	K	Joback Method
tc	819.40	K	Joback Method
tf	377.49	K	Joback Method
vc	0.603	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	395.72	J/mol×K	609.20	Joback Method
cpg	409.76	J/mol×K	644.23	Joback Method
cpg	422.99	J/mol×K	679.27	Joback Method
cpg	435.44	J/mol×K	714.30	Joback Method
cpg	447.11	J/mol×K	749.33	Joback Method
cpg	458.03	J/mol×K	784.36	Joback Method
cpg	468.21	J/mol×K	819.40	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=U374483&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U374483&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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