

# Benzamide, 4-methoxy-N-butyl-N-2-ethylhexyl-

<b>Inchi:</b>	InChI=1S/C20H33NO2/c1-5-8-10-17(7-3)16-21(15-9-6-2)20(22)18-11-13-19(23-4)14-12-
<b>InchiKey:</b>	MIYWIBVFCQFICA-UHFFFAOYSA-N
<b>Formula:</b>	C20H33NO2
<b>SMILES:</b>	CCCCC(CC)CN(CCCC)C(=O)c1ccc(OC)cc1
<b>Mol. weight [g/mol]:</b>	319.48

## Physical Properties

Property code	Value	Unit	Source
gf	94.72	kJ/mol	Joback Method
hf	-413.62	kJ/mol	Joback Method
hfus	43.49	kJ/mol	Joback Method
hvap	73.86	kJ/mol	Joback Method
log10ws	-5.68		Crippen Method
logp	5.154		Crippen Method
mvol	286.320	ml/mol	McGowan Method
pc	1303.29	kPa	Joback Method
rinpol	2956.00		NIST Webbook
rinpol	2956.00		NIST Webbook
tb	776.95	K	Joback Method
tc	969.88	K	Joback Method
tf	443.73	K	Joback Method
vc	1.083	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	868.90	J/molxK	776.95	Joback Method
cpg	887.34	J/molxK	809.10	Joback Method
cpg	904.68	J/molxK	841.26	Joback Method
cpg	920.98	J/molxK	873.41	Joback Method
cpg	936.26	J/molxK	905.57	Joback Method
cpg	950.57	J/molxK	937.72	Joback Method
cpg	963.95	J/molxK	969.88	Joback Method

# Sources

<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=U415910&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U415910&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>

# 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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