

# Benzamide, 4-methyl-N-butyl-N-octyl-

<b>Inchi:</b>	InChI=1S/C20H33NO/c1-4-6-8-9-10-11-17-21(16-7-5-2)20(22)19-14-12-18(3)13-15-19/h
<b>InchiKey:</b>	LEEZXKADHGANNK-UHFFFAOYSA-N
<b>Formula:</b>	C20H33NO
<b>SMILES:</b>	CCCCCCCCN(CCCC)C(=O)c1ccc(C)cc1
<b>Mol. weight [g/mol]:</b>	303.48

## Physical Properties

Property code	Value	Unit	Source
gf	202.16	kJ/mol	Joback Method
hf	-276.12	kJ/mol	Joback Method
hfus	45.83	kJ/mol	Joback Method
hvap	71.84	kJ/mol	Joback Method
log10ws	-6.28		Crippen Method
logp	5.598		Crippen Method
mvol	280.450	ml/mol	McGowan Method
pc	1311.80	kPa	Joback Method
rinpol	2999.00		NIST Webbook
rinpol	2999.00		NIST Webbook
tb	754.97	K	Joback Method
tc	945.36	K	Joback Method
tf	436.50	K	Joback Method
vc	1.071	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	837.43	J/molxK	754.97	Joback Method
cpg	856.07	J/molxK	786.70	Joback Method
cpg	873.65	J/molxK	818.43	Joback Method
cpg	890.24	J/molxK	850.16	Joback Method
cpg	905.89	J/molxK	881.89	Joback Method
cpg	920.64	J/molxK	913.63	Joback Method
cpg	934.54	J/molxK	945.36	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=U415926&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U415926&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>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>rlnpol:</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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