

# Benzamide, 4-butyl-N-octyl-

<b>Inchi:</b>	InChI=1S/C19H31NO/c1-3-5-7-8-9-10-16-20-19(21)18-14-12-17(13-15-18)11-6-4-2/h12-
<b>InchiKey:</b>	NEVRXRUEJPCMTR-UHFFFAOYSA-N
<b>Formula:</b>	C19H31NO
<b>SMILES:</b>	CCCCCCCCNC(=O)c1ccc(CCCC)cc1
<b>Mol. weight [g/mol]:</b>	289.46

## Physical Properties

Property code	Value	Unit	Source
gf	172.35	kJ/mol	Joback Method
hf	-269.54	kJ/mol	Joback Method
hfus	45.32	kJ/mol	Joback Method
hvap	74.01	kJ/mol	Joback Method
log10ws	-6.39		Crippen Method
logp	5.120		Crippen Method
mvol	266.360	ml/mol	McGowan Method
pc	1423.99	kPa	Joback Method
rinpol	2517.00		NIST Webbook
rinpol	2517.00		NIST Webbook
tb	769.82	K	Joback Method
tc	964.44	K	Joback Method
tf	445.42	K	Joback Method
vc	1.032	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	799.27	J/mol×K	769.82	Joback Method
cpg	816.88	J/mol×K	802.26	Joback Method
cpg	833.47	J/mol×K	834.69	Joback Method
cpg	849.09	J/mol×K	867.13	Joback Method
cpg	863.78	J/mol×K	899.57	Joback Method
cpg	877.60	J/mol×K	932.01	Joback Method
cpg	890.58	J/mol×K	964.44	Joback Method

# Sources

<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</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>
<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=U407455&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U407455&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>hvp:</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>rinp:</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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