

# Benzamide, 4-butyl-N-(hept-2-yl)-

<b>Inchi:</b>	InChI=1S/C18H29NO/c1-4-6-8-9-15(3)19-18(20)17-13-11-16(12-14-17)10-7-5-2/h11-15H
<b>InchiKey:</b>	HOYVROFMCOGLJY-UHFFFAOYSA-N
<b>Formula:</b>	C18H29NO
<b>SMILES:</b>	CCCCC(C)NC(=O)c1ccc(CCCC)cc1
<b>Mol. weight [g/mol]:</b>	275.43

## Physical Properties

Property code	Value	Unit	Source
gf	161.49	kJ/mol	Joback Method
hf	-254.18	kJ/mol	Joback Method
hfus	39.20	kJ/mol	Joback Method
hvap	71.39	kJ/mol	Joback Method
log10ws	-6.08		Crippen Method
logp	4.728		Crippen Method
mvol	252.270	ml/mol	McGowan Method
pc	1542.71	kPa	Joback Method
rinpol	2271.00		NIST Webbook
rinpol	2271.00		NIST Webbook
tb	746.50	K	Joback Method
tc	944.50	K	Joback Method
tf	419.15	K	Joback Method
vc	0.971	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	742.07	J/mol×K	746.50	Joback Method
cpg	759.66	J/mol×K	779.50	Joback Method
cpg	776.22	J/mol×K	812.50	Joback Method
cpg	791.79	J/mol×K	845.50	Joback Method
cpg	806.42	J/mol×K	878.50	Joback Method
cpg	820.14	J/mol×K	911.50	Joback Method
cpg	833.01	J/mol×K	944.50	Joback Method

# Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=U407451&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U407451&amp;Units=SI</a>
<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.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>

# 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>hvpap:</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>rinppl:</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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