

# Benzamide, 2-methyl-N-butyl-N-pentyl-

<b>Inchi:</b>	InChI=1S/C17H27NO/c1-4-6-10-14-18(13-7-5-2)17(19)16-12-9-8-11-15(16)3/h8-9,11-12
<b>InchiKey:</b>	QDAHTHYFGZTORP-UHFFFAOYSA-N
<b>Formula:</b>	C17H27NO
<b>SMILES:</b>	CCCCCN(CCCC)C(=O)c1ccccc1C
<b>Mol. weight [g/mol]:</b>	261.40

## Physical Properties

Property code	Value	Unit	Source
gf	176.90	kJ/mol	Joback Method
hf	-214.20	kJ/mol	Joback Method
hfus	38.06	kJ/mol	Joback Method
hvap	65.16	kJ/mol	Joback Method
log10ws	-5.02		Crippen Method
logp	4.428		Crippen Method
mvol	238.180	ml/mol	McGowan Method
pc	1635.13	kPa	Joback Method
rinpol	2817.00		NIST Webbook
rinpol	2817.00		NIST Webbook
tb	686.33	K	Joback Method
tc	879.80	K	Joback Method
tf	402.69	K	Joback Method
vc	0.903	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	665.78	J/mol×K	686.33	Joback Method
cpg	683.67	J/mol×K	718.58	Joback Method
cpg	700.55	J/mol×K	750.82	Joback Method
cpg	716.47	J/mol×K	783.07	Joback Method
cpg	731.47	J/mol×K	815.31	Joback Method
cpg	745.59	J/mol×K	847.56	Joback Method
cpg	758.88	J/mol×K	879.80	Joback Method

# Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=U415732&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U415732&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>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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