

# Phenylacetamide, N,N-dibutyl-

<b>Inchi:</b>	InChI=1S/C16H25NO/c1-3-5-12-17(13-6-4-2)16(18)14-15-10-8-7-9-11-15/h7-11H,3-6,12
<b>InchiKey:</b>	KNKHTVMCLHDUNM-UHFFFAOYSA-N
<b>Formula:</b>	C16H25NO
<b>SMILES:</b>	CCCCN(CCCC)C(=O)Cc1ccccc1
<b>Mol. weight [g/mol]:</b>	247.38

## Physical Properties

Property code	Value	Unit	Source
gf	178.11	kJ/mol	Joback Method
hf	-182.09	kJ/mol	Joback Method
hfus	35.86	kJ/mol	Joback Method
hvap	62.28	kJ/mol	Joback Method
log10ws	-3.97		Crippen Method
logp	3.658		Crippen Method
mvol	224.090	ml/mol	McGowan Method
pc	1792.42	kPa	Joback Method
rinpol	1885.00		NIST Webbook
rinpol	1885.00		NIST Webbook
tb	658.47	K	Joback Method
tc	853.00	K	Joback Method
tf	378.90	K	Joback Method
vc	0.848	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	610.93	J/mol×K	658.47	Joback Method
cpg	628.70	J/mol×K	690.89	Joback Method
cpg	645.44	J/mol×K	723.31	Joback Method
cpg	661.20	J/mol×K	755.73	Joback Method
cpg	676.02	J/mol×K	788.16	Joback Method
cpg	689.97	J/mol×K	820.58	Joback Method
cpg	703.07	J/mol×K	853.00	Joback Method

# Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=U308406&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U308406&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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