

# N-Benzoyl-dl-alanine

<b>Other names:</b>	Benzoyl-dl-«alpha»-alanine Benzoyl-dl-alanine dl-N-Benzoylalanine DL-Alanine, N-benzoyl- Alanine, N-benzoyl-, DL- DL-n-Benzoyl-«alpha»-alanine DI-n-benzoyl-alpha-alanine
<b>Inchi:</b>	InChI=1S/C10H11NO3/c1-7(10(13)14)11-9(12)8-5-3-2-4-6-8/h2-7H,1H3,(H,11,12)(H,13,14)
<b>InchiKey:</b>	UAQVHNZEONHPQG-UHFFFAOYSA-N
<b>Formula:</b>	C10H11NO3
<b>SMILES:</b>	CC(NC(=O)c1ccccc1)C(=O)O
<b>Mol. weight [g/mol]:</b>	193.20
<b>CAS:</b>	1205-02-3

## Physical Properties

Property code	Value	Unit	Source
gf	-161.98	kJ/mol	Joback Method
hf	-342.40	kJ/mol	Joback Method
hfus	24.56	kJ/mol	Joback Method
hvap	76.35	kJ/mol	Joback Method
log10ws	-1.86		Crippen Method
logp	0.889		Crippen Method
mcvol	146.990	ml/mol	McGowan Method
pc	3867.48	kPa	Joback Method
tb	704.53	K	Joback Method
tc	915.36	K	Joback Method
tf	427.22	K	Joback Method
vc	0.547	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	387.05	J/molxK	704.53	Joback Method
cpg	397.07	J/molxK	739.67	Joback Method

cpg	406.36	J/mol×K	774.81	Joback Method
cpg	414.95	J/mol×K	809.95	Joback Method
cpg	422.88	J/mol×K	845.08	Joback Method
cpg	430.19	J/mol×K	880.22	Joback Method
cpg	436.90	J/mol×K	915.36	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=C1205023&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C1205023&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>

## 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>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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