

# D-Alanine, N-(4-butylbenzoyl)-, pentyl ester

**Inchi:** InChI=1S/C19H29NO3/c1-4-6-8-14-23-19(22)15(3)20-18(21)17-12-10-16(11-13-17)9-7-5  
**InchiKey:** XFUWYBSDJXIXSA-UHFFFAOYSA-N  
**Formula:** C19H29NO3  
**SMILES:** CCCCCOC(=O)C(C)NC(=O)c1ccc(CCCC)cc1  
**Mol. weight [g/mol]:** 319.44

## Physical Properties

Property code	Value	Unit	Source
gf	-64.01	kJ/mol	Joback Method
hf	-519.62	kJ/mol	Joback Method
hfus	44.58	kJ/mol	Joback Method
hvap	82.78	kJ/mol	Joback Method
log10ws	-5.36		Crippen Method
logp	3.881		Crippen Method
mvol	273.800	ml/mol	McGowan Method
pc	1483.85	kPa	Joback Method
rinpol	2523.00		NIST Webbook
rinpol	2523.00		NIST Webbook
tb	845.67	K	Joback Method
tc	1050.28	K	Joback Method
tf	502.58	K	Joback Method
vc	1.050	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	849.47	J/molxK	845.67	Joback Method
cpg	865.17	J/molxK	879.77	Joback Method
cpg	879.77	J/molxK	913.87	Joback Method
cpg	893.29	J/molxK	947.97	Joback Method
cpg	905.79	J/molxK	982.08	Joback Method
cpg	917.29	J/molxK	1016.18	Joback Method
cpg	927.84	J/molxK	1050.28	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=U354099&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U354099&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307l">http://pubs.acs.org/doi/abs/10.1021/ci990307l</a>
<b>Crippen Method:</b>	<a href="https://www.cheméo.com/doc/models/crippen_log10ws">https://www.cheméo.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>rinpola:</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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