

# D-Alanine, N-(3-anisoyl)-, butyl ester

<b>Inchi:</b>	InChI=1S/C15H21NO4/c1-4-5-9-20-15(18)11(2)16-14(17)12-7-6-8-13(10-12)19-3/h6-8,10
<b>InchiKey:</b>	GVDHEXQUZZYHQX-UHFFFAOYSA-N
<b>Formula:</b>	C15H21NO4
<b>SMILES:</b>	CCCCOC(=O)C(C)NC(=O)c1cccc(OC)c1
<b>Mol. weight [g/mol]:</b>	279.33

## Physical Properties

Property code	Value	Unit	Source
gf	-202.69	kJ/mol	Joback Method
hf	-569.28	kJ/mol	Joback Method
hfus	35.41	kJ/mol	Joback Method
hvap	76.28	kJ/mol	Joback Method
log10ws	-3.42		Crippen Method
logp	2.157		Crippen Method
mcvol	223.310	ml/mol	McGowan Method
pc	2012.70	kPa	Joback Method
rinqol	2240.00		NIST Webbook
tb	776.57	K	Joback Method
tc	984.18	K	Joback Method
tf	479.73	K	Joback Method
vc	0.845	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	649.30	J/molxK	776.57	Joback Method
cpg	663.62	J/molxK	811.17	Joback Method
cpg	676.92	J/molxK	845.77	Joback Method
cpg	689.21	J/molxK	880.38	Joback Method
cpg	700.50	J/molxK	914.98	Joback Method
cpg	710.81	J/molxK	949.58	Joback Method
cpg	720.14	J/molxK	984.18	Joback Method

# Sources

<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.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>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=U354043&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U354043&amp;Units=SI</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>mccvol:</b>	McGowan's characteristic volume
<b>pc:</b>	Critical Pressure
<b>rinpol:</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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