

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

<b>Inchi:</b>	InChI=1S/C16H23NO4/c1-4-5-6-11-21-16(19)12(2)17-15(18)13-7-9-14(20-3)10-8-13/h7-
<b>InchiKey:</b>	QFSAGTSZZGPCMA-UHFFFAOYSA-N
<b>Formula:</b>	C16H23NO4
<b>SMILES:</b>	CCCCCOC(=O)C(C)NC(=O)c1ccc(OC)cc1
<b>Mol. weight [g/mol]:</b>	293.36

## Physical Properties

Property code	Value	Unit	Source
gf	-194.27	kJ/mol	Joback Method
hf	-589.92	kJ/mol	Joback Method
hfus	38.00	kJ/mol	Joback Method
hvap	78.51	kJ/mol	Joback Method
log10ws	-3.84		Crippen Method
logp	2.547		Crippen Method
mvol	237.400	ml/mol	McGowan Method
pc	1849.92	kPa	Joback Method
rinpol	2302.00		NIST Webbook
rinpol	2302.00		NIST Webbook
tb	799.45	K	Joback Method
tc	1005.61	K	Joback Method
tf	491.00	K	Joback Method
vc	0.900	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	705.23	J/molxK	799.45	Joback Method
cpg	719.81	J/molxK	833.81	Joback Method
cpg	733.34	J/molxK	868.17	Joback Method
cpg	745.82	J/molxK	902.53	Joback Method
cpg	757.27	J/molxK	936.89	Joback Method
cpg	767.71	J/molxK	971.25	Joback Method
cpg	777.16	J/molxK	1005.61	Joback Method

# Sources

<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>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=U348489&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U348489&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>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

Latest version available from:

<https://www.chemeo.com/cid/118-306-1/D-Alanine-N-4-anisoyl-pentyl-ester.pdf>

Generated by Cheméo on 2024-04-29 22:50:34.716228597 +0000 UTC m=+16720283.636805908.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.