

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

**Inchi:** InChI=1S/C18H27NO4/c1-4-5-6-7-8-12-23-18(21)14(2)19-17(20)15-10-9-11-16(13-15)22  
**InchiKey:** IMGRSSZOHYX AFC-UHFFFAOYSA-N  
**Formula:** C18H27NO4  
**SMILES:** CCCCCCOC(=O)C(C)NC(=O)c1cccc(OC)c1  
**Mol. weight [g/mol]:** 321.41

## Physical Properties

Property code	Value	Unit	Source
gf	-177.43	kJ/mol	Joback Method
hf	-631.20	kJ/mol	Joback Method
hfus	43.18	kJ/mol	Joback Method
hvap	82.96	kJ/mol	Joback Method
log10ws	-4.68		Crippen Method
logp	3.327		Crippen Method
mvol	265.580	ml/mol	McGowan Method
pc	1578.46	kPa	Joback Method
rinpol	2543.00		NIST Webbook
rinpol	2543.00		NIST Webbook
tb	845.21	K	Joback Method
tc	1050.30	K	Joback Method
tf	513.54	K	Joback Method
vc	1.012	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	819.83	J/molxK	845.21	Joback Method
cpg	834.84	J/molxK	879.39	Joback Method
cpg	848.71	J/molxK	913.57	Joback Method
cpg	861.47	J/molxK	947.76	Joback Method
cpg	873.14	J/molxK	981.94	Joback Method
cpg	883.73	J/molxK	1016.12	Joback Method
cpg	893.27	J/molxK	1050.30	Joback Method

# Sources

<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=U354046&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U354046&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.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>

# 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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