

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

Inchi:	InChI=1S/C22H35NO4/c1-4-5-6-7-8-9-10-11-12-17-27-22(25)18(2)23-21(24)19-13-15-20
InchiKey:	RZBZNVSVSJRRP-UHFFFAOYSA-N
Formula:	C22H35NO4
SMILES:	CCCCCCCCCCCCOC(=O)C(C)NC(=O)c1ccc(OC)cc1
Mol. weight [g/mol]:	377.52

## Physical Properties

Property code	Value	Unit	Source
gf	-143.75	kJ/mol	Joback Method
hf	-713.76	kJ/mol	Joback Method
hfus	53.54	kJ/mol	Joback Method
hvap	91.86	kJ/mol	Joback Method
log10ws	-6.35		Crippen Method
logp	4.888		Crippen Method
mcvol	321.940	ml/mol	McGowan Method
pc	1188.24	kPa	Joback Method
rinpol	2926.00		NIST Webbook
rinpol	2926.00		NIST Webbook
tb	936.73	K	Joback Method
tc	1148.47	K	Joback Method
tf	558.62	K	Joback Method
vc	1.236	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1057.99	J/molxK	936.73	Joback Method
cpg	1073.72	J/molxK	972.02	Joback Method
cpg	1088.10	J/molxK	1007.31	Joback Method
cpg	1101.18	J/molxK	1042.60	Joback Method
cpg	1112.98	J/molxK	1077.89	Joback Method
cpg	1123.54	J/molxK	1113.18	Joback Method
cpg	1132.89	J/molxK	1148.47	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=U348495&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U348495&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>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

Latest version available from:

<https://www.chemeo.com/cid/38-057-7/D-Alanine-N-4-anisoyl-undecyl-ester.pdf>

Generated by Cheméo on 2024-04-19 19:10:42.873485839 +0000 UTC m=+15843091.794063151.

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