

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

<b>Inchi:</b>	InChI=1S/C23H37NO4/c1-4-5-6-7-8-9-10-11-12-13-18-28-23(26)19(2)24-22(25)20-14-16
<b>InchiKey:</b>	FRVKJBPYBQJXOV-UHFFFAOYSA-N
<b>Formula:</b>	C23H37NO4
<b>SMILES:</b>	CCCCCCCCCCCCOC(=O)C(C)NC(=O)c1ccc(OC)cc1
<b>Mol. weight [g/mol]:</b>	391.54

## Physical Properties

Property code	Value	Unit	Source
gf	-135.33	kJ/mol	Joback Method
hf	-734.40	kJ/mol	Joback Method
hfus	56.13	kJ/mol	Joback Method
hvap	94.09	kJ/mol	Joback Method
log10ws	-6.77		Crippen Method
logp	5.278		Crippen Method
mvol	336.030	ml/mol	McGowan Method
pc	1113.34	kPa	Joback Method
rinpol	3010.00		NIST Webbook
rinpol	3010.00		NIST Webbook
tb	959.61	K	Joback Method
tc	1175.17	K	Joback Method
tf	569.89	K	Joback Method
vc	1.292	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1119.01	J/molxK	959.61	Joback Method
cpg	1134.94	J/molxK	995.54	Joback Method
cpg	1149.45	J/molxK	1031.46	Joback Method
cpg	1162.58	J/molxK	1067.39	Joback Method
cpg	1174.37	J/molxK	1103.32	Joback Method
cpg	1184.87	J/molxK	1139.25	Joback Method
cpg	1194.11	J/molxK	1175.17	Joback Method

# Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=U348496&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U348496&amp;Units=SI</a>
<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.cheméo.com/doc/models/crippen_log10ws">https://www.cheméo.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>

# 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.cheméo.com/cid/99-230-7/D-Alanine-N-4-anisoyl-dodecyl-ester.pdf>

Generated by Cheméo on 2024-04-19 14:28:58.830351688 +0000 UTC m=+15826187.750929003.

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