

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

<b>Inchi:</b>	InChI=1S/C17H25NO4/c1-12(2)6-5-11-22-17(20)13(3)18-16(19)14-7-9-15(21-4)10-8-14/
<b>InchiKey:</b>	MRKSZAQGUPAGIV-UHFFFAOYSA-N
<b>Formula:</b>	C17H25NO4
<b>SMILES:</b>	COc1ccc(C(=O)NC(C)C(=O)OCCCC(C)C)cc1
<b>Mol. weight [g/mol]:</b>	307.38

## Physical Properties

Property code	Value	Unit	Source
gf	-188.29	kJ/mol	Joback Method
hf	-615.84	kJ/mol	Joback Method
hfus	37.06	kJ/mol	Joback Method
hvap	80.35	kJ/mol	Joback Method
log10ws	-4.02		Crippen Method
logp	2.793		Crippen Method
mvol	251.490	ml/mol	McGowan Method
pc	1717.45	kPa	Joback Method
rinpol	2354.00		NIST Webbook
rinpol	2354.00		NIST Webbook
tb	821.89	K	Joback Method
tc	1029.57	K	Joback Method
tf	487.27	K	Joback Method
vc	0.951	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	762.65	J/mol×K	821.89	Joback Method
cpg	777.62	J/mol×K	856.50	Joback Method
cpg	791.45	J/mol×K	891.12	Joback Method
cpg	804.18	J/mol×K	925.73	Joback Method
cpg	815.81	J/mol×K	960.34	Joback Method
cpg	826.36	J/mol×K	994.96	Joback Method
cpg	835.86	J/mol×K	1029.57	Joback Method

# Sources

<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=U348490&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U348490&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.cheméo.com/doc/models/crippen_log10ws">https://www.cheméo.com/doc/models/crippen_log10ws</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>h vap:</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>r in pol:</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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