

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

Inchi:	InChI=1S/C19H29NO4/c1-4-5-6-7-8-9-14-24-19(22)15(2)20-18(21)16-10-12-17(23-3)13-
InchiKey:	YJSACINDSSKXRZ-UHFFFAOYSA-N
Formula:	C19H29NO4
SMILES:	CCCCCCCCOC(=O)C(C)NC(=O)c1ccc(OC)cc1
Mol. weight [g/mol]:	335.44

## Physical Properties

Property code	Value	Unit	Source
gf	-169.01	kJ/mol	Joback Method
hf	-651.84	kJ/mol	Joback Method
hfus	45.77	kJ/mol	Joback Method
hvap	85.19	kJ/mol	Joback Method
log10ws	-5.10		Crippen Method
logp	3.717		Crippen Method
mcvol	279.670	ml/mol	McGowan Method
pc	1464.61	kPa	Joback Method
rinpol	2608.00		NIST Webbook
tb	868.09	K	Joback Method
tc	1073.67	K	Joback Method
tf	524.81	K	Joback Method
vc	1.069	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	878.35	J/molxK	868.09	Joback Method
cpg	893.55	J/molxK	902.35	Joback Method
cpg	907.56	J/molxK	936.62	Joback Method
cpg	920.42	J/molxK	970.88	Joback Method
cpg	932.15	J/molxK	1005.14	Joback Method
cpg	942.77	J/molxK	1039.41	Joback Method
cpg	952.31	J/molxK	1073.67	Joback Method

# Sources

<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=U348492&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U348492&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>

## 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>rinpol:</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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