

# D-Alanine, N-allyloxycarbonyl-, nonyl ester

<b>Inchi:</b>	InChI=1S/C16H29NO4/c1-4-6-7-8-9-10-11-13-20-15(18)14(3)17-16(19)21-12-5-2/h5,14H
<b>InchiKey:</b>	SJWWDMSJBZJYRK-UHFFFAOYSA-N
<b>Formula:</b>	C16H29NO4
<b>SMILES:</b>	C=CCOC(=O)NC(C)C(=O)OCCCCCCCCC
<b>Mol. weight [g/mol]:</b>	299.41

## Physical Properties

Property code	Value	Unit	Source
gf	-209.21	kJ/mol	Joback Method
hf	-689.55	kJ/mol	Joback Method
hfus	43.07	kJ/mol	Joback Method
hvap	74.90	kJ/mol	Joback Method
log10ws	-4.38		Crippen Method
logp	3.581		Crippen Method
mcvol	256.860	ml/mol	McGowan Method
pc	1480.43	kPa	Joback Method
rinpol	2042.00		NIST Webbook
rinpol	2042.00		NIST Webbook
tb	764.47	K	Joback Method
tc	948.61	K	Joback Method
tf	450.30	K	Joback Method
vc	0.990	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	769.58	J/molxK	764.47	Joback Method
cpg	785.39	J/molxK	795.16	Joback Method
cpg	800.31	J/molxK	825.85	Joback Method
cpg	814.35	J/molxK	856.54	Joback Method
cpg	827.53	J/molxK	887.23	Joback Method
cpg	839.85	J/molxK	917.92	Joback Method
cpg	851.34	J/molxK	948.61	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=U347732&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U347732&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307I">http://pubs.acs.org/doi/abs/10.1021/ci990307I</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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