

# D-Alanine, N-propargyloxycarbonyl-, isohexyl ester

Inchi:	InChI=1S/C13H21NO4/c1-5-8-18-13(16)14-11(4)12(15)17-9-6-7-10(2)3/h1,10-11H,6-9H2
InchiKey:	AYVQOFBIFHCAHI-UHFFFAOYSA-N
Formula:	C13H21NO4
SMILES:	C#CCOC(=O)NC(C)C(=O)OCCCC(C)C
Mol. weight [g/mol]:	255.31

## Physical Properties

Property code	Value	Unit	Source
gf	-101.68	kJ/mol	Joback Method
hf	-466.44	kJ/mol	Joback Method
hfus	36.03	kJ/mol	Joback Method
hvap	68.36	kJ/mol	Joback Method
log10ws	-2.82		Crippen Method
logp	1.714		Crippen Method
mcvol	210.290	ml/mol	McGowan Method
pc	2071.76	kPa	Joback Method
rinpola	1725.00		NIST Webbook
rinpola	1725.00		NIST Webbook
tb	688.83	K	Joback Method
tc	881.46	K	Joback Method
tf	450.22	K	Joback Method
vc	0.796	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	578.59	J/molxK	688.83	Joback Method
cpg	592.91	J/molxK	720.94	Joback Method
cpg	606.46	J/molxK	753.04	Joback Method
cpg	619.22	J/molxK	785.15	Joback Method
cpg	631.22	J/molxK	817.25	Joback Method
cpg	642.46	J/molxK	849.36	Joback Method
cpg	652.95	J/molxK	881.46	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=U347741&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U347741&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>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

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