

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

<b>Inchi:</b>	InChI=1S/C15H29NO4/c1-11(2)8-7-9-19-13(17)12(3)16-14(18)20-10-15(4,5)6/h11-12H,7
<b>InchiKey:</b>	QOFOSMUMEOVLLS-UHFFFAOYSA-N
<b>Formula:</b>	C15H29NO4
<b>SMILES:</b>	CC(C)CCCOC(=O)C(C)NC(=O)OCC(C)(C)C
<b>Mol. weight [g/mol]:</b>	287.40

## Physical Properties

Property code	Value	Unit	Source
gf	-305.07	kJ/mol	Joback Method
hf	-808.37	kJ/mol	Joback Method
hfus	30.82	kJ/mol	Joback Method
hvap	71.66	kJ/mol	Joback Method
log10ws	-3.62		Crippen Method
logp	3.127		Crippen Method
mcvol	247.070	ml/mol	McGowan Method
pc	1577.21	kPa	Joback Method
rinpol	1799.00		NIST Webbook
rinpol	1799.00		NIST Webbook
tb	741.24	K	Joback Method
tc	931.02	K	Joback Method
tf	428.21	K	Joback Method
vc	0.935	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	740.31	J/molxK	741.24	Joback Method
cpg	756.70	J/molxK	772.87	Joback Method
cpg	772.14	J/molxK	804.50	Joback Method
cpg	786.64	J/molxK	836.13	Joback Method
cpg	800.23	J/molxK	867.76	Joback Method
cpg	812.92	J/molxK	899.39	Joback Method
cpg	824.76	J/molxK	931.02	Joback Method

# Sources

<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.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=U347763&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U347763&amp;Units=SI</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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