

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

<b>Inchi:</b>	InChI=1S/C14H27NO4/c1-10(11(16)18-8-13(2,3)4)15-12(17)19-9-14(5,6)7/h10H,8-9H2,1
<b>InchiKey:</b>	OBVBERBSSOUWFJ-UHFFFAOYSA-N
<b>Formula:</b>	C14H27NO4
<b>SMILES:</b>	CC(NC(=O)OCC(C)(C)C)C(=O)OCC(C)(C)C
<b>Mol. weight [g/mol]:</b>	273.37

## Physical Properties

Property code	Value	Unit	Source
gf	-308.21	kJ/mol	Joback Method
hf	-791.20	kJ/mol	Joback Method
hfus	24.34	kJ/mol	Joback Method
hvap	68.53	kJ/mol	Joback Method
log10ws	-3.20		Crippen Method
logp	2.736		Crippen Method
mcvol	232.980	ml/mol	McGowan Method
pc	1720.31	kPa	Joback Method
rinpol	1635.00		NIST Webbook
rinpol	1635.00		NIST Webbook
tb	715.57	K	Joback Method
tc	911.04	K	Joback Method
tf	434.36	K	Joback Method
vc	0.875	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	685.92	J/molxK	715.57	Joback Method
cpg	702.15	J/molxK	748.15	Joback Method
cpg	717.38	J/molxK	780.73	Joback Method
cpg	731.66	J/molxK	813.31	Joback Method
cpg	745.03	J/molxK	845.88	Joback Method
cpg	757.52	J/molxK	878.46	Joback Method
cpg	769.16	J/molxK	911.04	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=U347777&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U347777&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>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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