

# DL-Alanyl-DL-alanine, N,N'-dimethyl-N'-(3-chloropropoxycarbonyl)-, octyl ester

InChI: InChI=1S/C20H37ClN2O5/c1-6-7-8-9-10-11-14-27-19(25)17(3)22(4)18(24)16(2)23(5)20(6)13  
InChIKey: MBULMBGHZLUKIL-UHFFFAOYSA-N

Formula: C20H37ClN2O5

SMILES: CCCCCCOC(=O)C(C)N(C)C(=O)C(C)N(C)C(=O)OCCCCI

Mol. weight [g/mol]: 420.97

## Physical Properties

Property code	Value	Unit	Source
gf	-274.49	kJ/mol	Joback Method
hf	-949.55	kJ/mol	Joback Method
hfus	57.92	kJ/mol	Joback Method
hvap	92.87	kJ/mol	Joback Method
log10ws	-4.19		Crippen Method
logp	3.823		Crippen Method
mvol	341.310	ml/mol	McGowan Method
pc	1105.21	kPa	Joback Method
rinpol	2286.00		NIST Webbook
rinpol	2286.00		NIST Webbook
tb	924.88	K	Joback Method
tc	1132.32	K	Joback Method
tf	574.27	K	Joback Method
vc	1.282	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1107.38	J/molxK	924.88	Joback Method
cpg	1123.43	J/molxK	959.45	Joback Method
cpg	1138.19	J/molxK	994.03	Joback Method
cpg	1151.70	J/molxK	1028.60	Joback Method
cpg	1164.00	J/molxK	1063.17	Joback Method
cpg	1175.13	J/molxK	1097.74	Joback Method
cpg	1185.15	J/molxK	1132.32	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=U393237&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U393237&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>h vap:</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>r in pol:</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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