

# D-Alanine, N-(2-chlorobenzoyl)-, tetradecyl ester

Inchi:	InChI=1S/C24H38ClNO3/c1-3-4-5-6-7-8-9-10-11-12-13-16-19-29-24(28)20(2)26-23(27)2
InchiKey:	HTXJPUJDKHLVNZ-UHFFFAOYSA-N
Formula:	C24H38ClNO3
SMILES:	CCCCCCCCCCCCCOC(=O)C(C)NC(=O)c1ccccc1Cl
Mol. weight [g/mol]:	424.02

## Physical Properties

Property code	Value	Unit	Source
gf	-33.84	kJ/mol	Joback Method
hf	-638.56	kJ/mol	Joback Method
hfus	61.73	kJ/mol	Joback Method
hvap	98.29	kJ/mol	Joback Method
log10ws	-8.17		Crippen Method
logp	6.703		Crippen Method
mvol	356.490	ml/mol	McGowan Method
pc	1031.91	kPa	Joback Method
rinpol	3166.00		NIST Webbook
rinpol	3166.00		NIST Webbook
tb	997.50	K	Joback Method
tc	1221.23	K	Joback Method
tf	588.85	K	Joback Method
vc	1.379	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1177.08	J/molxK	997.50	Joback Method
cpg	1192.85	J/molxK	1034.79	Joback Method
cpg	1207.27	J/molxK	1072.08	Joback Method
cpg	1220.42	J/molxK	1109.36	Joback Method
cpg	1232.37	J/molxK	1146.65	Joback Method
cpg	1243.17	J/molxK	1183.94	Joback Method
cpg	1252.91	J/molxK	1221.23	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=U354081&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U354081&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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