

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

<b>Inchi:</b>	InChI=1S/C16H22ClNO3/c1-11(2)7-6-10-21-16(20)12(3)18-15(19)13-8-4-5-9-14(13)17/h
<b>InchiKey:</b>	OCACXILNDDMFHB-UHFFFAOYSA-N
<b>Formula:</b>	C16H22ClNO3
<b>SMILES:</b>	CC(C)CCCOC(=O)C(C)NC(=O)c1ccccc1Cl
<b>Mol. weight [g/mol]:</b>	311.80

## Physical Properties

Property code	Value	Unit	Source
gf	-103.64	kJ/mol	Joback Method
hf	-478.72	kJ/mol	Joback Method
hfus	37.48	kJ/mol	Joback Method
hvap	80.09	kJ/mol	Joback Method
log10ws	-4.58		Crippen Method
logp	3.438		Crippen Method
mvol	243.770	ml/mol	McGowan Method
pc	1830.98	kPa	Joback Method
rinpol	2284.00		NIST Webbook
rinpol	2284.00		NIST Webbook
tb	814.02	K	Joback Method
tc	1027.40	K	Joback Method
tf	483.69	K	Joback Method
vc	0.925	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	703.99	J/mol×K	814.02	Joback Method
cpg	718.01	J/mol×K	849.58	Joback Method
cpg	730.97	J/mol×K	885.15	Joback Method
cpg	742.90	J/mol×K	920.71	Joback Method
cpg	753.84	J/mol×K	956.27	Joback Method
cpg	763.83	J/mol×K	991.83	Joback Method
cpg	772.90	J/mol×K	1027.40	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=U354072&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U354072&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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