

# D-Alanine, N-(3-chloro-2-fluorobenzoyl)-, ethyl ester

<b>Inchi:</b>	InChI=1S/C12H13ClFNO3/c1-3-18-12(17)7(2)15-11(16)8-5-4-6-9(13)10(8)14/h4-7H,3H2
<b>InchiKey:</b>	OBRHTKOAKPUZBJ-UHFFFAOYSA-N
<b>Formula:</b>	C12H13ClFNO3
<b>SMILES:</b>	CCOC(=O)C(C)NC(=O)c1cccc(Cl)c1F
<b>Mol. weight [g/mol]:</b>	273.69

## Physical Properties

Property code	Value	Unit	Source
gf	-339.32	kJ/mol	Joback Method
hf	-598.46	kJ/mol	Joback Method
hfus	33.34	kJ/mol	Joback Method
hvap	71.42	kJ/mol	Joback Method
log10ws	-3.48		Crippen Method
logp	2.160		Crippen Method
mvol	189.180	ml/mol	McGowan Method
pc	2448.32	kPa	Joback Method
rinpol	1927.00		NIST Webbook
rinpol	1927.00		NIST Webbook
tb	727.19	K	Joback Method
tc	939.88	K	Joback Method
tf	466.72	K	Joback Method
vc	0.726	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	493.51	J/mol×K	727.19	Joback Method
cpg	505.24	J/mol×K	762.64	Joback Method
cpg	516.14	J/mol×K	798.09	Joback Method
cpg	526.22	J/mol×K	833.53	Joback Method
cpg	535.51	J/mol×K	868.98	Joback Method
cpg	544.00	J/mol×K	904.43	Joback Method
cpg	551.73	J/mol×K	939.88	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=U348333&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U348333&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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