

# D-Alanine, N-(2,6-difluoro-3-methylbenzoyl)-, undecyl ester

<b>Inchi:</b>	InChI=1S/C22H33F2NO3/c1-4-5-6-7-8-9-10-11-12-15-28-22(27)17(3)25-21(26)19-18(23)
<b>InchiKey:</b>	WHNZBRHFCKPBQL-UHFFFAOYSA-N
<b>Formula:</b>	C22H33F2NO3
<b>SMILES:</b>	CCCCCCCCCOC(=O)C(C)NC(=O)c1c(F)ccc(C)c1F
<b>Mol. weight [g/mol]:</b>	397.50

## Physical Properties

Property code	Value	Unit	Source
gf	-447.63	kJ/mol	Joback Method
hf	-996.70	kJ/mol	Joback Method
hfus	57.73	kJ/mol	Joback Method
hvap	89.14	kJ/mol	Joback Method
log10ws	-7.37		Crippen Method
logp	5.466		Crippen Method
mvol	319.610	ml/mol	McGowan Method
pc	1108.15	kPa	Joback Method
rinpol	2780.00		NIST Webbook
rinpol	2780.00		NIST Webbook
tb	922.81	K	Joback Method
tc	1130.16	K	Joback Method
tf	562.61	K	Joback Method
vc	1.254	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1041.42	J/molxK	922.81	Joback Method
cpg	1057.11	J/molxK	957.37	Joback Method
cpg	1071.58	J/molxK	991.93	Joback Method
cpg	1084.87	J/molxK	1026.49	Joback Method
cpg	1097.02	J/molxK	1061.05	Joback Method
cpg	1108.07	J/molxK	1095.61	Joback Method
cpg	1118.04	J/molxK	1130.16	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=U348392&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U348392&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>

# 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>hvp:</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>rinp:</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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