

# D-Alanine, N-(3-fluoro-5-trifluoromethylbenzoyl)-, undecyl ester

InChI: InChI=1S/C22H31F4NO3/c1-3-4-5-6-7-8-9-10-11-12-30-21(29)16(2)27-20(28)17-13-18(2)  
InChIKey: OWWBAHNFHMLXII-UHFFFAOYSA-N

Formula: C22H31F4NO3

SMILES: CCCCCCCCCCOC(=O)C(C)NC(=O)c1cc(F)cc(C(F)(F)F)c1

Mol. weight [g/mol]: 433.48

## Physical Properties

Property code	Value	Unit	Source
gf	-824.78	kJ/mol	Joback Method
hf	-1386.20	kJ/mol	Joback Method
hfus	56.87	kJ/mol	Joback Method
hvap	85.55	kJ/mol	Joback Method
log10ws	-7.67		Crippen Method
logp	6.037		Crippen Method
mcvol	323.150	ml/mol	McGowan Method
pc	1067.97	kPa	Joback Method
rinpol	2443.00		NIST Webbook
rinpol	2443.00		NIST Webbook
tb	913.14	K	Joback Method
tc	1118.03	K	Joback Method
tf	553.69	K	Joback Method
vc	1.280	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1056.69	J/molxK	913.14	Joback Method
cpg	1071.99	J/molxK	947.29	Joback Method
cpg	1086.17	J/molxK	981.44	Joback Method
cpg	1099.31	J/molxK	1015.58	Joback Method
cpg	1111.44	J/molxK	1049.73	Joback Method
cpg	1122.65	J/molxK	1083.88	Joback Method
cpg	1132.99	J/molxK	1118.03	Joback Method

# Sources

<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</a>
<b>Crippen Method:</b>	<a href="https://www.cheméo.com/doc/models/crippen_log10ws">https://www.cheméo.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=U347810&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U347810&amp;Units=SI</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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