

# D-Alanine, N-(2-fluoro-3-trifluoromethylbenzoyl)-, tetradecyl ester

InChI: CCCCCCCCCCCCCOC(=O)C(C)NC(=O)c1cccc(C(F)(F)F)c1F  
InChIKey: FRIUVJJOYMRMQ-UHFFFAOYSA-N

Formula: C<sub>25</sub>H<sub>37</sub>F<sub>4</sub>NO<sub>3</sub>

SMILES: CCCCCCCCCCCCCOC(=O)C(C)NC(=O)c1cccc(C(F)(F)F)c1F

Mol. weight [g/mol]: 475.56

## Physical Properties

Property code	Value	Unit	Source
gf	-799.52	kJ/mol	Joback Method
hf	-1448.12	kJ/mol	Joback Method
hfus	64.64	kJ/mol	Joback Method
hvap	92.23	kJ/mol	Joback Method
log10ws	-8.92		Crippen Method
logp	7.207		Crippen Method
mvol	365.420	ml/mol	McGowan Method
pc	892.13	kPa	Joback Method
rinpol	2882.00		NIST Webbook
rinpol	2882.00		NIST Webbook
tb	981.78	K	Joback Method
tc	1205.47	K	Joback Method
tf	587.50	K	Joback Method
vc	1.448	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1239.87	J/mol×K	981.78	Joback Method
cpg	1256.59	J/mol×K	1019.06	Joback Method
cpg	1271.99	J/mol×K	1056.34	Joback Method
cpg	1286.15	J/mol×K	1093.63	Joback Method
cpg	1299.17	J/mol×K	1130.91	Joback Method
cpg	1311.13	J/mol×K	1168.19	Joback Method
cpg	1322.14	J/mol×K	1205.47	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=U348425&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U348425&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>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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