

# D-Alanine, N-(3-fluoro-4-trifluoromethylbenzoyl)-, tridecyl

Inchi:  
ester

InChI=1S/C24H35F4NO3/c1-3-4-5-6-7-8-9-10-11-12-13-16-32-23(31)18(2)29-22(30)19-1

InchiKey:

JCRQFHBQZWGTRD-UHFFFAOYSA-N

Formula:

C24H35F4NO3

SMILES:

CCCCCCCCCCCCOC(=O)C(C)NC(=O)c1ccc(C(F)(F)F)c(F)c1

Mol. weight [g/mol]:

461.53

## Physical Properties

Property code	Value	Unit	Source
gf	-807.94	kJ/mol	Joback Method
hf	-1427.48	kJ/mol	Joback Method
hfus	62.05	kJ/mol	Joback Method
hvap	90.00	kJ/mol	Joback Method
log10ws	-8.50		Crippen Method
logp	6.817		Crippen Method
mvol	351.330	ml/mol	McGowan Method
pc	945.58	kPa	Joback Method
rinpol	2733.00		NIST Webbook
rinpol	2733.00		NIST Webbook
tb	958.90	K	Joback Method
tc	1175.24	K	Joback Method
tf	576.23	K	Joback Method
vc	1.391	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1178.25	J/molxK	958.90	Joback Method
cpg	1194.46	J/molxK	994.96	Joback Method
cpg	1209.41	J/molxK	1031.01	Joback Method
cpg	1223.21	J/molxK	1067.07	Joback Method
cpg	1235.91	J/molxK	1103.13	Joback Method
cpg	1247.60	J/molxK	1139.18	Joback Method
cpg	1258.37	J/molxK	1175.24	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=U347789&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U347789&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.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.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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