

# D-Alanine, N-(2-fluoro-5-trifluoromethylbenzoyl)-, decyl

Inchi:  
ester

InChI=1S/C21H29F4NO3/c1-3-4-5-6-7-8-9-10-13-29-20(28)15(2)26-19(27)17-14-16(21)(2

InchiKey:

WTOGYXVDBNBNSD-UHFFFAOYSA-N

Formula:

C21H29F4NO3

SMILES:

CCCCCCCCCOC(=O)C(C)NC(=O)c1cc(C(F)(F)F)ccc1F

Mol. weight [g/mol]:

419.45

## Physical Properties

Property code	Value	Unit	Source
gf	-833.20	kJ/mol	Joback Method
hf	-1365.56	kJ/mol	Joback Method
hfus	54.28	kJ/mol	Joback Method
hvap	83.33	kJ/mol	Joback Method
log10ws	-7.25		Crippen Method
logp	5.647		Crippen Method
mcvol	309.060	ml/mol	McGowan Method
pc	1138.27	kPa	Joback Method
rinqol	2437.00		NIST Webbook
tb	890.26	K	Joback Method
tc	1090.89	K	Joback Method
tf	542.42	K	Joback Method
vc	1.224	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	996.83	J/molxK	890.26	Joback Method
cpg	1011.74	J/molxK	923.70	Joback Method
cpg	1025.58	J/molxK	957.14	Joback Method
cpg	1038.41	J/molxK	990.58	Joback Method
cpg	1050.29	J/molxK	1024.02	Joback Method
cpg	1061.27	J/molxK	1057.46	Joback Method
cpg	1071.41	J/molxK	1090.89	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=U348352&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U348352&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307I">http://pubs.acs.org/doi/abs/10.1021/ci990307I</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>hvac:</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>mccol:</b>	McGowan's characteristic volume
<b>pc:</b>	Critical Pressure
<b>rinpol:</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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