

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

InChI: InChI=1S/C27H41F4NO3/c1-3-4-5-6-7-8-9-10-11-12-13-14-15-16-20-35-26(34)21(2)32-2  
InChIKey: HQMUMQLPQKZIDE-UHFFFAOYSA-N

Formula: C27H41F4NO3

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

Mol. weight [g/mol]: 503.61

## Physical Properties

Property code	Value	Unit	Source
gf	-782.68	kJ/mol	Joback Method
hf	-1489.40	kJ/mol	Joback Method
hfus	69.82	kJ/mol	Joback Method
hvap	96.68	kJ/mol	Joback Method
log10ws	-9.76		Crippen Method
logp	7.987		Crippen Method
mvol	393.600	ml/mol	McGowan Method
pc	797.98	kPa	Joback Method
rinpol	3061.00		NIST Webbook
rinpol	3061.00		NIST Webbook
tb	1027.54	K	Joback Method
tc	1269.63	K	Joback Method
tf	610.04	K	Joback Method
vc	1.560	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1364.57	J/molxK	1027.54	Joback Method
cpg	1382.49	J/molxK	1067.89	Joback Method
cpg	1398.90	J/molxK	1108.24	Joback Method
cpg	1413.91	J/molxK	1148.58	Joback Method
cpg	1427.65	J/molxK	1188.93	Joback Method
cpg	1440.25	J/molxK	1229.28	Joback Method
cpg	1451.83	J/molxK	1269.63	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=U348427&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U348427&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.cheméo.com/doc/models/crippen_log10ws">https://www.cheméo.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>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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