

# «beta»-Alanine, N-(3-trifluoromethylbenzoyl)-, hexadecyl ester

Inchi:	InChI=1S/C27H42F3NO3/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-21-34-25(32)19-20-31-2
InchiKey:	VRPAJFDLSKFMNL-UHFFFAOYSA-N
Formula:	C27H42F3NO3
SMILES:	CCCCCCCCCCCCCCCCOC(=O)CCNC(=O)c1cccc(C(F)(F)F)c1
Mol. weight [g/mol]:	485.62

## Physical Properties

Property code	Value	Unit	Source
gf	-575.80	kJ/mol	Joback Method
hf	-1276.54	kJ/mol	Joback Method
hfus	70.65	kJ/mol	Joback Method
hvap	97.22	kJ/mol	Joback Method
log10ws	-9.32		Crippen Method
logp	7.850		Crippen Method
mcvol	391.830	ml/mol	McGowan Method
pc	821.95	kPa	Joback Method
tb	1023.73	K	Joback Method
tc	1262.40	K	Joback Method
tf	611.93	K	Joback Method
vc	1.548	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1358.38	J/molxK	1023.73	Joback Method
cpg	1376.51	J/molxK	1063.51	Joback Method
cpg	1393.19	J/molxK	1103.29	Joback Method
cpg	1408.57	J/molxK	1143.07	Joback Method
cpg	1422.76	J/molxK	1182.84	Joback Method
cpg	1435.89	J/molxK	1222.62	Joback Method
cpg	1448.09	J/molxK	1262.40	Joback Method

# Sources

<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>
<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=U321598&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U321598&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>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>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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