

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

<b>Inchi:</b>	InChI=1S/C23H34F3NO3/c1-2-3-4-5-6-7-8-9-10-11-17-30-21(28)15-16-27-22(29)19-13-1
<b>InchiKey:</b>	IFQPWUYPEWAEOW-UHFFFAOYSA-N
<b>Formula:</b>	C23H34F3NO3
<b>SMILES:</b>	CCCCCCCCCCCCOC(=O)CCNC(=O)c1cccc(C(F)(F)F)c1
<b>Mol. weight [g/mol]:</b>	429.52

## Physical Properties

Property code	Value	Unit	Source
gf	-609.48	kJ/mol	Joback Method
hf	-1193.98	kJ/mol	Joback Method
hfus	60.29	kJ/mol	Joback Method
hvap	88.32	kJ/mol	Joback Method
log10ws	-7.64		Crippen Method
logp	6.289		Crippen Method
mvol	335.470	ml/mol	McGowan Method
pc	1037.90	kPa	Joback Method
rinpol	2868.00		NIST Webbook
rinpol	2868.00		NIST Webbook
tb	932.21	K	Joback Method
tc	1141.29	K	Joback Method
tf	566.85	K	Joback Method
vc	1.323	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1110.44	J/molxK	932.21	Joback Method
cpg	1126.42	J/molxK	967.06	Joback Method
cpg	1141.24	J/molxK	1001.90	Joback Method
cpg	1154.99	J/molxK	1036.75	Joback Method
cpg	1167.74	J/molxK	1071.60	Joback Method
cpg	1179.56	J/molxK	1106.44	Joback Method
cpg	1190.53	J/molxK	1141.29	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.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=U321595&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U321595&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>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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