

# «beta»-Alanine, N-(4-trifluoromethylbenzoyl)-, decyl ester

Inchi:	InChI=1S/C21H30F3NO3/c1-2-3-4-5-6-7-8-9-16-28-19(26)14-15-25-20(27)17-10-12-18(1
InchiKey:	ODMUXELDHHUTSA-UHFFFAOYSA-N
Formula:	C21H30F3NO3
SMILES:	CCCCCCCCCOC(=O)CCNC(=O)c1ccc(C(F)(F)F)cc1
Mol. weight [g/mol]:	401.46

## Physical Properties

Property code	Value	Unit	Source
gf	-626.32	kJ/mol	Joback Method
hf	-1152.70	kJ/mol	Joback Method
hfus	55.11	kJ/mol	Joback Method
hvap	83.87	kJ/mol	Joback Method
log10ws	-6.81		Crippen Method
logp	5.509		Crippen Method
mcvol	307.290	ml/mol	McGowan Method
pc	1179.28	kPa	Joback Method
rinpol	2614.00		NIST Webbook
rinpol	2614.00		NIST Webbook
tb	886.45	K	Joback Method
tc	1087.07	K	Joback Method
tf	544.31	K	Joback Method
vc	1.212	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	989.91	J/mol×K	886.45	Joback Method
cpg	1005.08	J/mol×K	919.89	Joback Method
cpg	1019.21	J/mol×K	953.32	Joback Method
cpg	1032.34	J/mol×K	986.76	Joback Method
cpg	1044.54	J/mol×K	1020.19	Joback Method
cpg	1055.86	J/mol×K	1053.63	Joback Method
cpg	1066.37	J/mol×K	1087.07	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=U321744&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U321744&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>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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