

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

<b>Inchi:</b>	InChI=1S/C18H24F3NO3/c1-2-3-4-5-6-12-25-16(23)10-11-22-17(24)14-8-7-9-15(13-14)1
<b>InchiKey:</b>	CHMUBIUEDBEBM-UHFFFAOYSA-N
<b>Formula:</b>	C18H24F3NO3
<b>SMILES:</b>	CCCCCCCOC(=O)CCNC(=O)c1cccc(C(F)(F)F)c1
<b>Mol. weight [g/mol]:</b>	359.38

## Physical Properties

Property code	Value	Unit	Source
gf	-651.58	kJ/mol	Joback Method
hf	-1090.78	kJ/mol	Joback Method
hfus	47.34	kJ/mol	Joback Method
hvap	77.19	kJ/mol	Joback Method
log10ws	-5.55		Crippen Method
logp	4.339		Crippen Method
mcvol	265.020	ml/mol	McGowan Method
pc	1452.35	kPa	Joback Method
rinsol	2330.00		NIST Webbook
tb	817.81	K	Joback Method
tc	1012.06	K	Joback Method
tf	510.50	K	Joback Method
vc	1.044	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	814.47	J/mol×K	817.81	Joback Method
cpg	828.63	J/mol×K	850.19	Joback Method
cpg	841.84	J/mol×K	882.56	Joback Method
cpg	854.15	J/mol×K	914.94	Joback Method
cpg	865.60	J/mol×K	947.31	Joback Method
cpg	876.23	J/mol×K	979.69	Joback Method
cpg	886.10	J/mol×K	1012.06	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=U321590&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U321590&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.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.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>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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