

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

Inchi:	InChI=1S/C14H16F3NO3/c1-2-8-21-12(19)6-7-18-13(20)10-4-3-5-11(9-10)14(15,16)17/h
InchiKey:	VDZVFBGKQYVOPY-UHFFFAOYSA-N
Formula:	C14H16F3NO3
SMILES:	CCCOC(=O)CCNC(=O)c1cccc(C(F)(F)F)c1
Mol. weight [g/mol]:	303.28

## Physical Properties

Property code	Value	Unit	Source
gf	-685.26	kJ/mol	Joback Method
hf	-1008.22	kJ/mol	Joback Method
hfus	36.98	kJ/mol	Joback Method
hvap	68.29	kJ/mol	Joback Method
log10ws	-3.88		Crippen Method
logp	2.778		Crippen Method
mcvol	208.660	ml/mol	McGowan Method
pc	1992.98	kPa	Joback Method
rinsol	1937.00		NIST Webbook
tb	726.29	K	Joback Method
tc	921.44	K	Joback Method
tf	465.42	K	Joback Method
vc	0.820	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	593.07	J/mol×K	726.29	Joback Method
cpg	605.84	J/mol×K	758.82	Joback Method
cpg	617.75	J/mol×K	791.34	Joback Method
cpg	628.84	J/mol×K	823.87	Joback Method
cpg	639.14	J/mol×K	856.39	Joback Method
cpg	648.68	J/mol×K	888.92	Joback Method
cpg	657.52	J/mol×K	921.44	Joback Method

# Sources

<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=U321585&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U321585&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>
<b>Joback Method:</b>	<a href="https://en.wikipedia.org/wiki/Joback_method">https://en.wikipedia.org/wiki/Joback_method</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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