

# «beta»-Alanine, N-(2,3,4-trifluorobenzoyl)-, isobutyl ester

<b>Inchi:</b>	InChI=1S/C14H16F3NO3/c1-8(2)7-21-11(19)5-6-18-14(20)9-3-4-10(15)13(17)12(9)16/h3
<b>InchiKey:</b>	NOKNZJXHGMMAUSJ-UHFFFAOYSA-N
<b>Formula:</b>	C14H16F3NO3
<b>SMILES:</b>	CC(C)COC(=O)CCNC(=O)c1ccc(F)c(F)c1F
<b>Mol. weight [g/mol]:</b>	303.28

## Physical Properties

Property code	Value	Unit	Source
gf	-709.80	kJ/mol	Joback Method
hf	-1027.69	kJ/mol	Joback Method
hfus	40.09	kJ/mol	Joback Method
hvap	70.52	kJ/mol	Joback Method
log10ws	-3.94		Crippen Method
logp	2.423		Crippen Method
mcvol	208.660	ml/mol	McGowan Method
pc	1921.98	kPa	Joback Method
rinpola	1912.00		NIST Webbook
rinpola	1912.00		NIST Webbook
tb	739.04	K	Joback Method
tc	931.13	K	Joback Method
tf	473.04	K	Joback Method
vc	0.825	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	589.02	J/mol×K	739.04	Joback Method
cpg	601.56	J/mol×K	771.06	Joback Method
cpg	613.31	J/mol×K	803.07	Joback Method
cpg	624.30	J/mol×K	835.09	Joback Method
cpg	634.53	J/mol×K	867.10	Joback Method
cpg	644.01	J/mol×K	899.12	Joback Method
cpg	652.75	J/mol×K	931.13	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.cheméo.com/doc/models/crippen_log10ws">https://www.cheméo.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=U321690&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U321690&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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