

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

<b>Inchi:</b>	InChI=1S/C19H26F3NO3/c1-2-3-4-5-6-7-8-13-26-16(24)11-12-23-19(25)14-9-10-15(20)1
<b>InchiKey:</b>	IYBGMAGHYHCDSZ-UHFFFAOYSA-N
<b>Formula:</b>	C19H26F3NO3
<b>SMILES:</b>	CCCCCCCCCOC(=O)CCNC(=O)c1ccc(F)c(F)c1F
<b>Mol. weight [g/mol]:</b>	373.41

## Physical Properties

Property code	Value	Unit	Source
gf	-665.26	kJ/mol	Joback Method
hf	-1125.61	kJ/mol	Joback Method
hfus	56.56	kJ/mol	Joback Method
hvap	82.04	kJ/mol	Joback Method
log10ws	-6.28		Crippen Method
logp	4.518		Crippen Method
mvol	279.110	ml/mol	McGowan Method
pc	1304.23	kPa	Joback Method
rinpol	2462.00		NIST Webbook
tb	853.88	K	Joback Method
tc	1048.62	K	Joback Method
tf	544.39	K	Joback Method
vc	1.111	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	869.44	J/mol×K	853.88	Joback Method
cpg	883.82	J/mol×K	886.34	Joback Method
cpg	897.22	J/mol×K	918.79	Joback Method
cpg	909.64	J/mol×K	951.25	Joback Method
cpg	921.13	J/mol×K	983.71	Joback Method
cpg	931.70	J/mol×K	1016.17	Joback Method
cpg	941.38	J/mol×K	1048.62	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=U321696&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U321696&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307I">http://pubs.acs.org/doi/abs/10.1021/ci990307I</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

Latest version available from:

<https://www.chemeo.com/cid/59-055-6/beta-Alanine-N-2-3-4-trifluorobenzoyl-nonyl-ester.pdf>

Generated by Cheméo on 2024-04-26 06:12:01.659001639 +0000 UTC m=+16401170.579578960.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.