

# «beta»-Alanine, n-pentafluoropropionyl-, butyl ester

Inchi:	InChI=1S/C10H14F5NO3/c1-2-3-6-19-7(17)4-5-16-8(18)9(11,12)10(13,14)15/h2-6H2,1H
InchiKey:	IQVGRJYBMJYVOK-UHFFFAOYSA-N
Formula:	C10H14F5NO3
SMILES:	CCCCOC(=O)CCNC(=O)C(F)(F)C(F)(F)F
Mol. weight [g/mol]:	291.22

## Physical Properties

Property code	Value	Unit	Source
gf	-1208.50	kJ/mol	Joback Method
hf	-1551.69	kJ/mol	Joback Method
hfus	31.71	kJ/mol	Joback Method
hvap	53.52	kJ/mol	Joback Method
log10ws	-2.81		Crippen Method
logp	2.034		Crippen Method
mcvol	179.600	ml/mol	McGowan Method
pc	1987.66	kPa	Joback Method
rinpola	1303.00		NIST Webbook
rinpola	1303.00		NIST Webbook
tb	598.42	K	Joback Method
tc	763.85	K	Joback Method
tf	385.00	K	Joback Method
vc	0.729	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	488.83	J/mol×K	598.42	Joback Method
cpg	500.68	J/mol×K	625.99	Joback Method
cpg	511.87	J/mol×K	653.56	Joback Method
cpg	522.41	J/mol×K	681.13	Joback Method
cpg	532.35	J/mol×K	708.71	Joback Method
cpg	541.70	J/mol×K	736.28	Joback Method
cpg	550.49	J/mol×K	763.85	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=U320950&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U320950&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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