

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

<b>Inchi:</b>	InChI=1S/C10H14F5NO3/c1-6(2)5-19-7(17)3-4-16-8(18)9(11,12)10(13,14)15/h6H,3-5H2
<b>InchiKey:</b>	QAUNVMSVKLBREU-UHFFFAOYSA-N
<b>Formula:</b>	C10H14F5NO3
<b>SMILES:</b>	CC(C)COC(=O)CCNC(=O)C(F)(F)C(F)(F)F
<b>Mol. weight [g/mol]:</b>	291.22

## Physical Properties

Property code	Value	Unit	Source
gf	-1210.94	kJ/mol	Joback Method
hf	-1556.97	kJ/mol	Joback Method
hfus	28.19	kJ/mol	Joback Method
hvap	53.13	kJ/mol	Joback Method
log10ws	-2.57		Crippen Method
logp	1.889		Crippen Method
mvol	179.600	ml/mol	McGowan Method
pc	2001.91	kPa	Joback Method
rinpol	1266.00		NIST Webbook
rinpol	1266.00		NIST Webbook
tb	597.98	K	Joback Method
tc	765.95	K	Joback Method
tf	370.00	K	Joback Method
vc	0.723	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	489.24	J/mol×K	597.98	Joback Method
cpg	501.32	J/mol×K	625.97	Joback Method
cpg	512.71	J/mol×K	653.97	Joback Method
cpg	523.43	J/mol×K	681.96	Joback Method
cpg	533.51	J/mol×K	709.96	Joback Method
cpg	542.99	J/mol×K	737.95	Joback Method
cpg	551.89	J/mol×K	765.95	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=U320949&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U320949&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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