

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

Inchi:	InChI=1S/C8H10F5NO3/c1-2-17-5(15)3-4-14-6(16)7(9,10)8(11,12)13/h2-4H2,1H3,(H,14,
InchiKey:	CKXSZRHWOWOWNM-UHFFFAOYSA-N
Formula:	C8H10F5NO3
SMILES:	CCOC(=O)CCNC(=O)C(F)(F)C(F)(F)F
Mol. weight [g/mol]:	263.16

## Physical Properties

Property code	Value	Unit	Source
gf	-1225.34	kJ/mol	Joback Method
hf	-1510.41	kJ/mol	Joback Method
hfus	26.53	kJ/mol	Joback Method
hvap	49.06	kJ/mol	Joback Method
log10ws	-1.97		Crippen Method
logp	1.253		Crippen Method
mcvol	151.420	ml/mol	McGowan Method
pc	2377.22	kPa	Joback Method
rinpola	886.00		NIST Webbook
tb	552.66	K	Joback Method
tc	719.44	K	Joback Method
tf	362.46	K	Joback Method
vc	0.617	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	393.64	J/mol×K	552.66	Joback Method
cpg	404.27	J/mol×K	580.46	Joback Method
cpg	414.28	J/mol×K	608.25	Joback Method
cpg	423.70	J/mol×K	636.05	Joback Method
cpg	432.54	J/mol×K	663.84	Joback Method
cpg	440.85	J/mol×K	691.64	Joback Method
cpg	448.63	J/mol×K	719.44	Joback Method

# Sources

<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>
<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=U320947&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U320947&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>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>mccvol:</b>	McGowan's characteristic volume
<b>pc:</b>	Critical Pressure
<b>rinpol:</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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