

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

<b>Inchi:</b>	InChI=1S/C15H24F5NO3/c1-2-3-4-5-6-7-8-11-24-12(22)9-10-21-13(23)14(16,17)15(18,1
<b>InchiKey:</b>	BLFGOOAXXPXMS-UHFFFAOYSA-N
<b>Formula:</b>	C15H24F5NO3
<b>SMILES:</b>	CCCCCCCCCOC(=O)CCNC(=O)C(F)(F)C(F)(F)F
<b>Mol. weight [g/mol]:</b>	361.35

## Physical Properties

Property code	Value	Unit	Source
gf	-1166.40	kJ/mol	Joback Method
hf	-1654.89	kJ/mol	Joback Method
hfus	44.66	kJ/mol	Joback Method
hvap	64.64	kJ/mol	Joback Method
log10ws	-4.91		Crippen Method
logp	3.984		Crippen Method
mcvol	250.050	ml/mol	McGowan Method
pc	1348.67	kPa	Joback Method
rinpol	1758.00		NIST Webbook
rinpol	1758.00		NIST Webbook
tb	712.82	K	Joback Method
tc	881.08	K	Joback Method
tf	441.35	K	Joback Method
vc	1.008	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	751.17	J/molxK	712.82	Joback Method
cpg	765.47	J/molxK	740.86	Joback Method
cpg	778.97	J/molxK	768.91	Joback Method
cpg	791.72	J/molxK	796.95	Joback Method
cpg	803.76	J/molxK	825.00	Joback Method
cpg	815.11	J/molxK	853.04	Joback Method
cpg	825.82	J/molxK	881.08	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=U320954&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U320954&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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