

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

Inchi:	InChI=1S/C24H42F5NO3/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-20-33-21(31)18-19
InchiKey:	XTGJXGBMVYSVER-UHFFFAOYSA-N
Formula:	C24H42F5NO3
SMILES:	CCCCCCCCCCCCCCCCCOC(=O)CCNC(=O)C(F)(F)C(F)(F)F
Mol. weight [g/mol]:	487.59

## Physical Properties

Property code	Value	Unit	Source
gf	-1090.62	kJ/mol	Joback Method
hf	-1840.65	kJ/mol	Joback Method
hfus	67.97	kJ/mol	Joback Method
hvap	84.68	kJ/mol	Joback Method
log10ws	-8.67		Crippen Method
logp	7.495		Crippen Method
mvol	376.860	ml/mol	McGowan Method
pc	777.21	kPa	Joback Method
rinpol	2632.00		NIST Webbook
rinpol	2632.00		NIST Webbook
tb	918.74	K	Joback Method
tc	1134.11	K	Joback Method
tf	542.78	K	Joback Method
vc	1.512	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1286.38	J/mol×K	918.74	Joback Method
cpg	1306.13	J/mol×K	954.63	Joback Method
cpg	1324.57	J/mol×K	990.53	Joback Method
cpg	1341.80	J/mol×K	1026.42	Joback Method
cpg	1357.94	J/mol×K	1062.32	Joback Method
cpg	1373.09	J/mol×K	1098.21	Joback Method
cpg	1387.35	J/mol×K	1134.11	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=U320962&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U320962&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>rinpolar:</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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