

# L-Isoleucine, n-pentafluoropropionyl-, heptadecyl ester

<b>Inchi:</b>	InChI=1S/C26H46F5NO3/c1-4-6-7-8-9-10-11-12-13-14-15-16-17-18-19-20-35-23(33)22(
<b>InchiKey:</b>	PTDFUKZESFXECJ-UHFFFAOYSA-N
<b>Formula:</b>	C26H46F5NO3
<b>SMILES:</b>	CCCCCCCCCCCCCCCCOC(=O)C(NC(=O)C(F)(F)C(F)(F)F)C(C)CC
<b>Mol. weight [g/mol]:</b>	515.64

## Physical Properties

Property code	Value	Unit	Source
gf	-1078.66	kJ/mol	Joback Method
hf	-1892.49	kJ/mol	Joback Method
hfus	66.11	kJ/mol	Joback Method
hvap	88.35	kJ/mol	Joback Method
log10ws	-9.38		Crippen Method
logp	8.130		Crippen Method
mvol	405.040	ml/mol	McGowan Method
pc	706.21	kPa	Joback Method
rmpol	2595.00		NIST Webbook
rmpol	2595.00		NIST Webbook
tb	963.62	K	Joback Method
tc	1195.91	K	Joback Method
tf	535.32	K	Joback Method
vc	1.613	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1413.61	J/molxK	963.62	Joback Method
cpg	1434.72	J/molxK	1002.34	Joback Method
cpg	1454.32	J/molxK	1041.05	Joback Method
cpg	1472.57	J/molxK	1079.77	Joback Method
cpg	1489.60	J/molxK	1118.48	Joback Method
cpg	1505.56	J/molxK	1157.20	Joback Method
cpg	1520.59	J/molxK	1195.91	Joback Method

# Sources

<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=U320876&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U320876&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>
<b>Joback Method:</b>	<a href="https://en.wikipedia.org/wiki/Joback_method">https://en.wikipedia.org/wiki/Joback_method</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>h vap:</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>r in pol:</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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