

# I-Leucine, n-heptafluorobutyryl-, pentyl ester

**Inchi:** InChI=1S/C15H22F7NO3/c1-4-5-6-7-26-11(24)10(8-9(2)3)23-12(25)13(16,17)14(18,19)1  
**InchiKey:** QAZPCVQSQWEHCF-UHFFFAOYSA-N  
**Formula:** C15H22F7NO3  
**SMILES:** CCCCCOC(=O)C(CC(C)C)NC(=O)C(F)(F)C(F)(F)C(F)(F)F  
**Mol. weight [g/mol]:** 397.33

## Physical Properties

Property code	Value	Unit	Source
gf	-1558.06	kJ/mol	Joback Method
hf	-2066.42	kJ/mol	Joback Method
hfus	36.36	kJ/mol	Joback Method
hvap	60.94	kJ/mol	Joback Method
log10ws	-5.09		Crippen Method
logp	4.084		Crippen Method
mcvol	253.590	ml/mol	McGowan Method
pc	1295.79	kPa	Joback Method
rinqol	1484.00		NIST Webbook
tb	707.25	K	Joback Method
tc	875.10	K	Joback Method
tf	414.95	K	Joback Method
vc	1.022	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	770.11	J/molxK	707.25	Joback Method
cpg	784.12	J/molxK	735.22	Joback Method
cpg	797.28	J/molxK	763.20	Joback Method
cpg	809.65	J/molxK	791.17	Joback Method
cpg	821.28	J/molxK	819.15	Joback Method
cpg	832.20	J/molxK	847.12	Joback Method
cpg	842.47	J/molxK	875.10	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=U320993&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U320993&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307I">http://pubs.acs.org/doi/abs/10.1021/ci990307I</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>

# 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>m cvol:</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

Latest version available from:

<https://www.chemeo.com/cid/44-171-3/l-Leucine-n-heptafluorobutyryl-pentyl-ester.pdf>

Generated by Cheméo on 2026-05-14 03:37:44.572398896 +0000 UTC m=+2495213.630481116.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.