

# I-Isoleucine, n-heptafluorobutyryl-, decyl ester

**Inchi:** InChI=1S/C20H32F7NO3/c1-4-6-7-8-9-10-11-12-13-31-16(29)15(14(3)5-2)28-17(30)18(2)  
**InchiKey:** NLXPXTFAQNQCDG-UHFFFAOYSA-N  
**Formula:** C20H32F7NO3  
**SMILES:** CCCCCCCCCOC(=O)C(NC(=O)C(F)(F)C(F)(F)C(F)(F)F)C(C)CC  
**Mol. weight [g/mol]:** 467.46

## Physical Properties

Property code	Value	Unit	Source
gf	-1515.96	kJ/mol	Joback Method
hf	-2169.62	kJ/mol	Joback Method
hfus	49.31	kJ/mol	Joback Method
hvap	72.07	kJ/mol	Joback Method
log10ws	-7.18		Crippen Method
logp	6.034		Crippen Method
mcvol	324.040	ml/mol	McGowan Method
pc	942.10	kPa	Joback Method
rinpol	1945.00		NIST Webbook
tb	821.65	K	Joback Method
tc	1005.93	K	Joback Method
tf	471.30	K	Joback Method
vc	1.302	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1057.39	J/molxK	821.65	Joback Method
cpg	1073.73	J/molxK	852.36	Joback Method
cpg	1089.06	J/molxK	883.08	Joback Method
cpg	1103.47	J/molxK	913.79	Joback Method
cpg	1117.01	J/molxK	944.51	Joback Method
cpg	1129.78	J/molxK	975.22	Joback Method
cpg	1141.83	J/molxK	1005.93	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=U320929&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U320929&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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