

# I-Isoleucine, n-pentafluoropropionyl-, octyl ester

Inchi:	InChI=1S/C17H28F5NO3/c1-4-6-7-8-9-10-11-26-14(24)13(12(3)5-2)23-15(25)16(18,19)1
InchiKey:	BEJLBMIUOWYOGI-UHFFFAOYSA-N
Formula:	C17H28F5NO3
SMILES:	CCCCCCCCOC(=O)C(NC(=O)C(F)(F)C(F)(F)F)C(C)CC
Mol. weight [g/mol]:	389.40

## Physical Properties

Property code	Value	Unit	Source
gf	-1154.44	kJ/mol	Joback Method
hf	-1706.73	kJ/mol	Joback Method
hfus	42.80	kJ/mol	Joback Method
hvap	68.32	kJ/mol	Joback Method
log10ws	-5.61		Crippen Method
logp	4.619		Crippen Method
mcvol	278.230	ml/mol	McGowan Method
pc	1189.88	kPa	Joback Method
rinpol	1737.00		NIST Webbook
tb	757.70	K	Joback Method
tc	932.46	K	Joback Method
tf	433.89	K	Joback Method
vc	1.109	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	865.20	J/molxK	757.70	Joback Method
cpg	880.62	J/molxK	786.83	Joback Method
cpg	895.15	J/molxK	815.95	Joback Method
cpg	908.83	J/molxK	845.08	Joback Method
cpg	921.71	J/molxK	874.21	Joback Method
cpg	933.83	J/molxK	903.33	Joback Method
cpg	945.23	J/molxK	932.46	Joback Method

# Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=U320870&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U320870&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</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>

# 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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