

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

Inchi:	InChI=1S/C25H42F7NO3/c1-4-6-7-8-9-10-11-12-13-14-15-16-17-18-36-21(34)20(19(3)5
InchiKey:	NJYLJZZERKHJFY-UHFFFAOYSA-N
Formula:	C25H42F7NO3
SMILES:	CCCCCCCCCCCCCCCCOC(=O)C(NC(=O)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(C)CC
Mol. weight [g/mol]:	537.59

## Physical Properties

Property code	Value	Unit	Source
gf	-1473.86	kJ/mol	Joback Method
hf	-2272.82	kJ/mol	Joback Method
hfus	62.26	kJ/mol	Joback Method
hvap	83.20	kJ/mol	Joback Method
log10ws	-9.28		Crippen Method
logp	7.985		Crippen Method
mvol	394.490	ml/mol	McGowan Method
pc	715.68	kPa	Joback Method
rinpol	2416.00		NIST Webbook
tb	936.05	K	Joback Method
tc	1159.12	K	Joback Method
tf	527.65	K	Joback Method
vc	1.581	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1363.92	J/molxK	936.05	Joback Method
cpg	1383.93	J/molxK	973.23	Joback Method
cpg	1402.61	J/molxK	1010.41	Joback Method
cpg	1420.12	J/molxK	1047.59	Joback Method
cpg	1436.61	J/molxK	1084.76	Joback Method
cpg	1452.21	J/molxK	1121.94	Joback Method
cpg	1467.09	J/molxK	1159.12	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=U320932&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U320932&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.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.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>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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