

# L-Phenylalanine, n-heptafluorobutyryl-, octadecyl ester

<b>Inchi:</b>	InChI=1S/C31H46F7NO3/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-16-20-23-42-27(40)26(2
<b>InchiKey:</b>	TXNIOFWTPLLHT-UHFFFAOYSA-N
<b>Formula:</b>	C31H46F7NO3
<b>SMILES:</b>	CCCCCCCCCCCCCCCCCOC(=O)C(Cc1ccccc1)NC(=O)C(F)(F)C(F)(F)C(F)(F)F
<b>Mol. weight [g/mol]:</b>	613.69

## Physical Properties

Property code	Value	Unit	Source
gf	-1308.49	kJ/mol	Joback Method
hf	-2154.85	kJ/mol	Joback Method
hfus	75.37	kJ/mol	Joback Method
hvap	99.22	kJ/mol	Joback Method
log10ws	-11.13		Crippen Method
logp	9.352		Crippen Method
mvol	455.270	ml/mol	McGowan Method
pc	627.82	kPa	Joback Method
rinpol	3241.00		NIST Webbook
rinpol	3241.00		NIST Webbook
tb	1100.45	K	Joback Method
tc	1392.90	K	Joback Method
tf	636.69	K	Joback Method
vc	1.815	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1640.13	J/molxK	1100.45	Joback Method
cpg	1662.83	J/molxK	1149.19	Joback Method
cpg	1684.36	J/molxK	1197.93	Joback Method
cpg	1705.14	J/molxK	1246.68	Joback Method
cpg	1725.55	J/molxK	1295.42	Joback Method
cpg	1746.00	J/molxK	1344.16	Joback Method
cpg	1766.89	J/molxK	1392.90	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=U321121&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U321121&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>

# 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>mcvol:</b>	McGowan's characteristic volume
<b>pc:</b>	Critical Pressure
<b>rinpola:</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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