

# (E,Z)-Farnesyl caproate

<b>Inchi:</b>	InChI=1S/C21H36O2/c1-6-7-8-15-21(22)23-17-16-20(5)14-10-13-19(4)12-9-11-18(2)3/h
<b>InchiKey:</b>	RLRVQTPROCYANT-GTCQVGLTSA-N
<b>Formula:</b>	C21H36O2
<b>SMILES:</b>	CCCCC(=O)OCC=C(C)CCC=C(C)CCC=C(C)C
<b>Mol. weight [g/mol]:</b>	320.51

## Physical Properties

Property code	Value	Unit	Source
gf	107.03	kJ/mol	Joback Method
hf	-399.28	kJ/mol	Joback Method
hfus	49.61	kJ/mol	Joback Method
hvap	71.61	kJ/mol	Joback Method
log10ws	-7.04		Crippen Method
logp	6.529		Crippen Method
mvol	301.290	ml/mol	McGowan Method
pc	1098.62	kPa	Joback Method
ripol	2447.00		NIST Webbook
ripol	2447.00		NIST Webbook
tb	768.29	K	Joback Method
tc	955.62	K	Joback Method
tf	341.47	K	Joback Method
vc	1.179	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	896.62	J/molxK	768.29	Joback Method
cpg	915.56	J/molxK	799.51	Joback Method
cpg	933.58	J/molxK	830.73	Joback Method
cpg	950.73	J/molxK	861.96	Joback Method
cpg	967.07	J/molxK	893.18	Joback Method
cpg	982.67	J/molxK	924.40	Joback Method
cpg	997.58	J/molxK	955.62	Joback Method

# Sources

<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>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=R517396&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R517396&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>mcvol:</b>	McGowan's characteristic volume
<b>pc:</b>	Critical Pressure
<b>ripol:</b>	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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