

# Senkyunolide J

<b>Inchi:</b>	InChI=1S/C12H18O4/c1-2-3-4-9-7-5-6-8(13)11(14)10(7)12(15)16-9/h8-9,11,13-14H,2-6H
<b>InchiKey:</b>	AXRIHSJZHOTGAE-UHFFFAOYSA-N
<b>Formula:</b>	C12H18O4
<b>SMILES:</b>	CCCCC1OC(=O)C2=C1CCC(O)C2O
<b>Mol. weight [g/mol]:</b>	226.27
<b>CAS:</b>	94530-86-6

## Physical Properties

Property code	Value	Unit	Source
gf	-344.00	kJ/mol	Joback Method
hf	-723.55	kJ/mol	Joback Method
hfus	33.99	kJ/mol	Joback Method
hvap	86.07	kJ/mol	Joback Method
log10ws	-2.21		Crippen Method
logp	0.914		Crippen Method
mcvol	173.100	ml/mol	McGowan Method
pc	2915.53	kPa	Joback Method
rinpol	1973.90		NIST Webbook
rinpol	1973.90		NIST Webbook
tb	783.83	K	Joback Method
tc	983.26	K	Joback Method
tf	488.31	K	Joback Method
vc	0.648	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	559.35	J/mol×K	783.83	Joback Method
cpg	572.19	J/mol×K	817.07	Joback Method
cpg	584.20	J/mol×K	850.31	Joback Method
cpg	595.41	J/mol×K	883.54	Joback Method
cpg	605.82	J/mol×K	916.78	Joback Method
cpg	615.46	J/mol×K	950.02	Joback Method
cpg	624.32	J/mol×K	983.26	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.cheméo.com/doc/models/crippen_log10ws">https://www.cheméo.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=C94530866&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C94530866&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>hvp:</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>rinp:</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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