

# Senkyunolide H

<b>Inchi:</b>	InChI=1S/C12H16O4/c1-2-3-4-9-7-5-6-8(13)11(14)10(7)12(15)16-9/h4,8,11,13-14H,2-3,5
<b>InchiKey:</b>	DQNGMIQSNXNGHOA-WTKPLQERSA-N
<b>Formula:</b>	C12H16O4
<b>SMILES:</b>	CCCC=C1OC(=O)C2=C1CCC(O)C2O
<b>Mol. weight [g/mol]:</b>	224.25
<b>CAS:</b>	94596-27-7

## Physical Properties

Property code	Value	Unit	Source
gf	-290.83	kJ/mol	Joback Method
hf	-627.18	kJ/mol	Joback Method
hfus	33.24	kJ/mol	Joback Method
hvap	87.17	kJ/mol	Joback Method
log10ws	-2.45		Crippen Method
logp	1.039		Crippen Method
mvol	168.800	ml/mol	McGowan Method
pc	3121.00	kPa	Joback Method
rinpol	2033.90		NIST Webbook
tb	795.14	K	Joback Method
tc	998.83	K	Joback Method
tf	502.91	K	Joback Method
vc	0.632	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	527.94	J/molxK	795.14	Joback Method
cpg	539.66	J/molxK	829.09	Joback Method
cpg	550.64	J/molxK	863.04	Joback Method
cpg	560.90	J/molxK	896.99	Joback Method
cpg	570.47	J/molxK	930.93	Joback Method
cpg	579.35	J/molxK	964.88	Joback Method
cpg	587.59	J/molxK	998.83	Joback Method

# Sources

<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=C94596277&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C94596277&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>
<b>Joback Method:</b>	<a href="https://en.wikipedia.org/wiki/Joback_method">https://en.wikipedia.org/wiki/Joback_method</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>h vap:</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>r in pol:</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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