

# «alpha»-Santonin

<b>Other names:</b>	(-)-Santonin (-)-Santonine (-)-«alpha»-Santonin (-)-À «alphaÂ»-Santonin (3S,3aS,5aS,9bS)-2,3,3a,4,5,5a,8,9b-octahydro-3,5a,9-trimethylnaphtho[1,2-b]furan-2,8-1,2,3,4,4a,7-Hexahydro-1-hydroxy-«alpha», 4a,8-trimethyl-7-oxo-2-naphthaleneacetic acid «gamma»-lactone 1,2,3,4,4a,7-Hexahydro-1-hydroxy-A«alphaÂ», 4a,8-trimethyl-7-oxo-2-naphthaleneacetic acid À «gammaÂ»-lactone 11-Epiisoeusantona-1,4-dienic acid, 6«alpha»-hydroxy-3-oxo-, «gamma»-lactone 11-Epiisoeusantona-1,4-dienic acid, 6À «alphaÂ»-hydroxy-3-oxo-, À «gammaÂ»-lactone Eudesma-1,4-dien-12-oic acid, 6«alpha»-hydroxy-3-oxo-, «gamma»-lactone, (11S)- Eudesma-1,4-dien-12-oic acid, 6À «alphaÂ»-hydroxy-3-oxo-, À «gammaÂ»-lactone, (11S)- NSC 4900 Naphtho(1,2-b)furan-2,8(3H,4H)-dione, 3a,5,5a,9b-tetrahydro-3,5a,9-trimethyl-, [3S,3aS,5aS,9bS]- Naphtho[1,2-b]furan-2,8(3H,4H)-dione, 3a,5,5a,9b-tetrahydro-3,5a,9-trimethyl-, [3S-(3«alpha»,3a«alpha»,5a«beta»,9b«beta»)]- Naphtho[1,2-b]furan-2,8(3H,4H)-dione, 3a,5,5a,9b-tetrahydro-3,5a,9-trimethyl-, [3S-(3À «alphaÂ»,3aÀ «alphaÂ»,5aÀ «betaÂ»,9bÀ «betaÂ»)]- Santonin Santoninic anhydride Semenen [3S-(3«alpha»,3a«alpha»,5a«beta»,9b«beta»)]-3a,5,5a,9b-Tetrahydro-3,5a,9-trimethylNa [3S-(3À «alphaÂ»,3aÀ «alphaÂ»,5aÀ «betaÂ»,9bÀ «betaÂ»)]-3a,5,5a,9b-Tetrahydro-3,5a, I-«alpha»-Santonin I-À «alphaÂ»-Santonin <b>Inchi:</b> InChI=1S/C15H18O3/c1-8-10-4-6-15(3)7-5-11(16)9(2)12(15)13(10)18-14(8)17/h5,7-8,10 <b>InchiKey:</b> XJHD MGJUR BV LLE-BOCCBSBMSA-N <b>Formula:</b> C15H18O3 <b>SMILES:</b> CC1=C2C3OC(=O)C(C)C3CCC2(C)C=CC1=O <b>Mol. weight [g/mol]:</b> 246.30 <b>CAS:</b> 481-06-1
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## Physical Properties

Property code	Value	Unit	Source
chs	-7884.30 ± 2.30	kJ/mol	NIST Webbook
gf	-94.57	kJ/mol	Joback Method
hf	-479.05	kJ/mol	Joback Method
hfs	-590.90 ± 2.30	kJ/mol	NIST Webbook
hfus	24.05	kJ/mol	Joback Method

hvap	62.86	kJ/mol	Joback Method
log10ws	-3.09		Estimated Solubility Method
log10ws	-3.09		Aqueous Solubility Prediction Method
logp	2.420		Crippen Method
mcvol	190.040	ml/mol	McGowan Method
pc	2372.59	kPa	Joback Method
rinpol	2117.00		NIST Webbook
tb	746.34	K	Joback Method
tc	1001.68	K	Joback Method
tf	507.78	K	Joback Method
vc	0.719	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	593.98	J/mol×K	746.34	Joback Method
cpg	614.21	J/mol×K	788.90	Joback Method
cpg	633.42	J/mol×K	831.45	Joback Method
cpg	651.77	J/mol×K	874.01	Joback Method
cpg	669.43	J/mol×K	916.57	Joback Method
cpg	686.54	J/mol×K	959.12	Joback Method
cpg	703.26	J/mol×K	1001.68	Joback Method

## Sources

<b>Estimated Solubility Method:</b>	<a href="http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt">http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt</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=C481061&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C481061&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>Joback Method:</b>	<a href="https://en.wikipedia.org/wiki/Joback_method">https://en.wikipedia.org/wiki/Joback_method</a>
<b>Aqueous Solubility Prediction Method:</b>	<a href="http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDataset002.xlsx">http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDataset002.xlsx</a>

## Legend

<b>chs:</b>	Standard solid enthalpy of combustion
<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>hfs:</b>	Solid phase 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>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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