«alpha»-Santonin

Other names:
(-)-Santonin
(-)-Santonine
(-)-«alpha»-Santonin
(-)-Â«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-Â«alphaÂ»,
4a,8-trimethyl-7-oxo-2-naphthaleneacetic acid Â«gammaÂ»-lactone
11-Epiisoeusantona-1,4-dienic acid, 6«alpha»-hydroxy-3-oxo-, «gamma»-lactone
11-Epiisoeusantona-1,4-dienic acid, 6Â«alphaÂ»-hydroxy-3-oxo-,
Â«gammaÂ»-lactone
Eudesma-1,4-dien-12-oic acid, 6«alpha»-hydroxy-3-oxo-, «gamma»-lactone,
(11S)-
Eudesma-1,4-dien-12-oic acid, 6Â«alphaÂ»-hydroxy-3-oxo-,
Â«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-(3Â«alphaÂ»,3aÂ«alphaÂ»,5aÂ«betaÂ»,9bÂ«betaÂ»)]-
Santonin
Santoninic anhydride
Semenen
[3S-(3«alpha»,3a«alpha»,5a«beta»,9b«beta»)]-3a,5,5a,9b-Tetrahydro-3,5a,9-trimethylna
[3S-(3Â«alphaÂ»,3aÂ«alphaÂ»,5aÂ«betaÂ»,9bÂ«betaÂ»)]-3a,5,5a,9b-Tetrahydro-3,5a,9
l-«alpha»-Santonin
l-Â«alphaÂ»-Santonin

Inchi: 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
InchiKey: XJHDMGJURBVLLE-BOCCBSBMSA-N
Formula: C15H18O3
SMILES: CC1=C2C3OC(=O)C(C)C3CCC2(C)C=CC1=O
Mol. weight [g/mol]: 246.30
CAS: 481-06-1

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

Aqueous Solubility Prediction Method: http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
Estimated Solubility Method: http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C481061&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Joback Method: https://en.wikipedia.org/wiki/Joback_method

Legend

chs:	Standard solid enthalpy of combustion
cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfs:	Solid phase enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume