Naphtho[1,2-b]furan-2,8(3H,4H)-dione, 3a,5,5a,9b-tetrahydro-3,5a,9-trimethyl-, [3R-(3«alpha»,3a«beta»,5a«alpha»,9b«alpha»)]-

Other names: Eudesma-1,4-dien-12-oic acid, 6«alpha»-hydroxy-3-oxo-, «gamma»-lactone, (12R)-
«beta»-Santonin
«beta»-Santonin-[3R-(3«alpha»,3a«beta»,5a«alpha»,9b«alpha»)]-
3a,5,5a,9b-tetrahydro-3,5a,9-trimethylnaphthalene

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-OMSPQPPYSA-N

Formula: C15H18O3

SMILES: CC1=C2C3OC(=O)C(C)C3CCC2(C)C=CC1=O

Mol. weight [g/mol]: 246.30

CAS: 481-07-2

Physical Properties

Property code	Value	Unit	Source
chs	-7887.80 ± 1.80	kJ/mol	NIST Webbook
gf	-94.57	kJ/mol	Joback Method
hf	-479.05	kJ/mol	Joback Method
hfs	-587.30 ± 1.80	kJ/mol	NIST Webbook
hfus	24.05	kJ/mol	Joback Method
hvap	62.86	kJ/mol	Joback Method
log10ws	-3.02		Crippen Method
logp	2.420		Crippen Method
mcvol	190.040	ml/mol	McGowan Method
pc	2372.59	kPa	Joback Method
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

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C481072&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume