Azuleno[4,5-b]furan-2,7-dione, 3,3a,4,5,9a,9b-hexahydro-3,6,9-trimethyl-, [3R-(3«alpha»,3a«beta»,9a«beta»,9b«alpha»)]-

Other names:	Guaia-4(10),3-dien-12-oic acid,6«alpha»-hydroxy-2-oxo-, «gamma»-lactone, (3R,3aS,9aS,9bS)- Achillin Azuleno[4,5-b]furan-2,7-dione, 3,3a,4,5,9a,9b-hexahydro-3,6,9-trimethyl-, (3R,3aS,9aS,9bS)- 3,6,9-Trimethyl-3,3a,4,5,9a,9b-hexahydroazuleno[4,5-b]furan-2,7-dione-, (3R,3aS,9aS,9bS)-
Inchi:	InChI=1S/C15H18O3/c1-7-4-5-10-9(3)15(17)18-14(10)13-8(2)6-11(16)12(7)13/h6,9-10,1
InchiKey:	BJPSSVHNEGMBDQ-UHFFFAOYSA-N
Formula:	C15H18O3
SMILES:	CC1=CC(=O)C2=C(C)CCC3C(C)C(=O)OC3C12
Mol. weight [g/mol]:	246.30
CAS:	5956-04-7

Physical Properties

Property code	Value	Unit	Source
gf	-98.71	kJ/mol	Joback Method
hf	-505.76	kJ/mol	Joback Method
hfus	29.96	kJ/mol	Joback Method
hvap	64.68	kJ/mol	Joback Method
log10ws	-3.02		Crippen Method
logp	2.420		Crippen Method
mcvol	190.040	ml/mol	McGowan Method
pc	2239.76	kPa	Joback Method
rinpol	2206.40		NIST Webbook
tb	751.08	K	Joback Method
tc	998.19	K	Joback Method
tf	496.40	K	Joback Method
vc	0.721	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	598.11	J/mol×K	751.08	Joback Method
cpg	617.46	J/mol×K	792.26	Joback Method
cpg	635.31	J/mol×K	833.45	Joback Method
cpg	651.65	J/mol×K	874.63	Joback Method

cpg	666.50	J/mol×K	915.82	Joback Method
cpg	679.87	J/mol×K	957.00	Joback Method
cpg	691.75	J/mol×K	998.19	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=C5956047&Units=SI

Legend

cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	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