Costunolide

Other names:	Germacra-1(10),4,11(13)-trien-12-oic acid, 6«alpha»-hydroxy-, «gamma»-lactone, (E,E)- Cyclodeca[b]furan-2(3H)-one, 3a,4,5,8,9,11a-hexahydro-6,10-dimethyl-3-methylene-, [3aS-(3aR*,6E,10E,11aS*)]- Costunolid Costus lactone (E,E)-6-«alpha»-Hydroxygermacra-1(10),4,11(13)-trien-12-oic acid «gamma»-lactone 6,10-Dimethyl-3-methylene-3a,4,5,8,9,11a-hexahydrocyclodeca[b]furan-2(3H)-one-, (3aS,6E,10E,11aR)- NSC 106404
Inchi:	InChI=1S/C15H20O2/c1-10-5-4-6-11(2)9-14-13(8-7-10)12(3)15(16)17-14/h5,9,13-14H,3-
InchiKey:	HRYLQFBHBWLLLL-GYIATTAWSA-N
Formula:	C15H20O2
SMILES:	C=C1C(=O)OC2C=C(C)CCC=C(C)CCC12
Mol. weight [g/mol]:	232.32
CAS:	553-21-9

Physical Properties

Property code	Value	Unit	Source
gf	-2.75	kJ/mol	Joback Method
hf	-343.29	kJ/mol	Joback Method
hfus	24.17	kJ/mol	Joback Method
hvap	60.84	kJ/mol	Joback Method
log10ws	-4.18		Crippen Method
logp	3.551		Crippen Method
mcvol	195.030	ml/mol	McGowan Method
pc	2191.78	kPa	Joback Method
tb	688.18	K	Joback Method
tc	932.76	K	Joback Method
tf	405.08	K	Joback Method
vc	0.718	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	560.07	J/mol×K	688.18	Joback Method
cpg	581.51	J/mol×K	728.94	Joback Method

cpg	601.37	J/mol×K	769.71	Joback Method
cpg	619.64	J/mol×K	810.47	Joback Method
cpg	636.29	J/mol×K	851.23	Joback Method
cpg	651.32	J/mol×K	892.00	Joback Method
cpg	664.71	J/mol×K	932.76	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=C553219&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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