Cyclodeca[b]furan-2(3H)-one, 3a,4,5,8,9,11a-hexahydro-3,6,10-trimethyl-, [3S-(3R*,3aR*,6E,10E,11aR*)]-

Other names: Germacra-1(10),4,11(13)-trien-12-oic acid, 6«alpha»-hydroxy-, «gamma»-lactone, (E,E)-; Costunolide; dihydro-

Cyclodeca[b]furan-2(3H)-one, 3a,4,5,8,9,11a-hexahydro-3,6,10-trimethyl-, [3S-(3R*,3aR*,6E,10E,11aS*)]-

Dihydrocostunolide

Inchi: InChI=1S/C15H22O2/c1-10-5-4-6-11(2)9-14-13(8-7-10)12(3)15(16)17-14/h5,9,12-14H,4,

InchiKey: OVDMFKGCVWVONO-GYIATTAWSA-N

Formula: C15H22O2

SMILES: CC1=CC2OC(=O)C(C)C2CCC(C)=CCC1

Mol. weight [g/mol]: 234.33

CAS: 2225-79-8

Physical Properties

Property code	Value	Unit	Source
gf	-63.54	kJ/mol	Joback Method
hf	-447.87	kJ/mol	Joback Method
hfus	26.40	kJ/mol	Joback Method
hvap	60.37	kJ/mol	Joback Method
log10ws	-4.09		Crippen Method
logp	3.631		Crippen Method
mcvol	199.330	ml/mol	McGowan Method
pc	2088.84	kPa	Joback Method
rinpol	1898.00		NIST Webbook
rinpol	1898.00		NIST Webbook
tb	684.35	K	Joback Method
tc	927.07	K	Joback Method
tf	387.16	K	Joback Method
vc	0.733	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	586.87	J/mol×K	684.35	Joback Method
cpg	609.93	J/mol×K	724.80	Joback Method
cpg	631.32	J/mol×K	765.26	Joback Method

cpg	651.02	J/mol×K	805.71	Joback Method
cpg	669.03	J/mol×K	846.17	Joback Method
cpg	685.32	J/mol×K	886.62	Joback Method
cpg	699.89	J/mol×K	927.07	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C2225798&Units=SI
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

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