Dehydrocostunolide

Inchi: InChI=1S/C15H18O2/c1-10-5-4-6-11(2)9-14-13(8-7-10)12(3)15(16)17-14/h5,8-9,14H,3-4
InchiKey: XBKBURWTMWWJNA-YHACVWLESA-N
Formula: C15H18O2
SMILES: C=C1C(=O)OC2C=C(C)CCC=C(C)CC=C12
Mol. weight [g/mol]: 230.30

Physical Properties

Property code	Value	Unit	Source
gf	25.29	kJ/mol	Joback Method
hf	-276.64	kJ/mol	Joback Method
hfus	23.93	kJ/mol	Joback Method
hvap	62.10	kJ/mol	Joback Method
log10ws	-4.28		Crippen Method
logp	3.471		Crippen Method
mcvol	190.730	ml/mol	McGowan Method
pc	2306.95	kPa	Joback Method
rinpol	1963.00		NIST Webbook
tb	696.99	K	Joback Method
tc	944.49	K	Joback Method
tf	422.60	K	Joback Method
vc	0.705	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	533.32	J/mol×K	696.99	Joback Method
cpg	552.91	J/mol×K	738.24	Joback Method
cpg	571.02	J/mol×K	779.49	Joback Method
cpg	587.63	J/mol×K	820.74	Joback Method
cpg	602.74	J/mol×K	861.99	Joback Method
cpg	616.33	J/mol×K	903.24	Joback Method
cpg	628.39	J/mol×K	944.49	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R340522&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