

14-Hydroxy-«beta»-caryophyllene acetate

Inchi:	InChI=1S/C17H26O2/c1-12-6-5-7-14(11-19-13(2)18)8-9-16-15(12)10-17(16,3)4/h7,15-16
InchiKey:	XLKYRVILZQUEJC-IAGRGRHTSA-N
Formula:	C17H26O2
SMILES:	<chem>C=C1CCC=C(COC(C)=O)CCC2C1CC2(C)C</chem>
Mol. weight [g/mol]:	262.39

Physical Properties

Property code	Value	Unit	Source
gf	-20.45	kJ/mol	Joback Method
hf	-398.76	kJ/mol	Joback Method
hfus	22.79	kJ/mol	Joback Method
hvap	62.93	kJ/mol	Joback Method
log10ws	-4.57		Crippen Method
logp	4.268		Crippen Method
mvol	227.510	ml/mol	McGowan Method
pc	1784.86	kPa	Joback Method
rinpol	1807.00		NIST Webbook
rinpol	1807.00		NIST Webbook
tb	698.35	K	Joback Method
tc	919.73	K	Joback Method
tf	418.41	K	Joback Method
vc	0.853	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	669.66	J/mol×K	698.35	Joback Method
cpg	691.18	J/mol×K	735.25	Joback Method
cpg	711.58	J/mol×K	772.14	Joback Method
cpg	730.98	J/mol×K	809.04	Joback Method
cpg	749.50	J/mol×K	845.93	Joback Method
cpg	767.26	J/mol×K	882.83	Joback Method
cpg	784.38	J/mol×K	919.73	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R618969&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

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
rinpola:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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