14-Acetoxy-«beta»-caryophyllene

Other names: 14-Acetoxy-«beta»-caryophyllene (=«alpha»-Betulenol acetate)
14-Acetoxy- «beta»-caryophyllene («alpha»-betulenol 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-AUWJEWJLSA-N
Formula: C17H26O2
SMILES: C=C1CCC=C(COC(C)=O)CCC2C1CC2(C)C
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
mcvol	227.510	ml/mol	McGowan Method
pc	1784.86	kPa	Joback Method
ripol	2272.00		NIST Webbook
ripol	2272.00		NIST Webbook
ripol	2310.00		NIST Webbook
ripol	2310.00		NIST Webbook
ripol	2272.00		NIST Webbook
ripol	2272.00		NIST Webbook
ripol	2272.00		NIST Webbook
ripol	2272.00		NIST Webbook
tb	698.35	K	Joback Method
tc	919.73	K	Joback Method
tf	418.41	K	Joback Method
vc	0.853	m3/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

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=R336122&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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