10-epi-«gamma»-eudesmol acetate

Inchi: InChI=1S/C17H28O2/c1-12-7-6-9-17(5)10-8-14(11-15(12)17)16(3,4)19-13(2)18/h14H,6-1
InchiKey: WJUQDFFDADGYQZ-WMLDXEAASA-N
Formula: C17H28O2
SMILES: CC(=O)OC(C)(C)C1CCC2(C)CCCC(C)=C2C1
Mol. weight [g/mol]: 264.40

Physical Properties

Property code	Value	Unit	Source
gf	-60.51	kJ/mol	Joback Method
hf	-476.72	kJ/mol	Joback Method
hfus	17.18	kJ/mol	Joback Method
hvap	62.28	kJ/mol	Joback Method
log10ws	-5.07		Crippen Method
logp	4.635		Crippen Method
mcvol	231.810	ml/mol	McGowan Method
pc	1774.35	kPa	Joback Method
rinpol	1741.00		NIST Webbook
rinpol	1741.00		NIST Webbook
tb	701.34	K	Joback Method
tc	927.04	K	Joback Method
tf	427.43	K	Joback Method
vc	0.867	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	691.67	J/mol×K	701.34	Joback Method
cpg	713.43	J/mol×K	738.96	Joback Method
cpg	734.03	J/mol×K	776.57	Joback Method
cpg	753.66	J/mol×K	814.19	Joback Method
cpg	772.46	J/mol×K	851.81	Joback Method
cpg	790.63	J/mol×K	889.42	Joback Method
cpg	808.32	J/mol×K	927.04	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R337214&Units=SI

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