11-Acetoxyeudesma-4-«alpha»-ol

Inchi: InChI=1S/C17H30O3/c1-12(18)20-15(2,3)13-7-10-16(4)8-6-9-17(5,19)14(16)11-13/h13-1
InchiKey: YJUFRKRDRWIRBO-WVKGIRLHSA-N
Formula: C17H30O3
SMILES: CC(=O)OC(C)(C)C1CCC2(C)CCCC(C)(O)C2C1
Mol. weight [g/mol]: 282.42

Physical Properties

Property code	Value	Unit	Source
gf	-228.94	kJ/mol	Joback Method
hf	-689.23	kJ/mol	Joback Method
hfus	16.66	kJ/mol	Joback Method
hvap	75.57	kJ/mol	Joback Method
log10ws	-4.35		Crippen Method
logp	3.686		Crippen Method
mcvol	241.980	ml/mol	McGowan Method
pc	1875.65	kPa	Joback Method
rinpol	1941.00		NIST Webbook
tb	775.30	K	Joback Method
tc	990.04	K	Joback Method
tf	477.87	K	Joback Method
vc	0.895	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	789.77	J/mol×K	775.30	Joback Method
cpg	810.57	J/mol×K	811.09	Joback Method
cpg	830.95	J/mol×K	846.88	Joback Method
cpg	851.12	J/mol×K	882.67	Joback Method
cpg	871.31	J/mol×K	918.46	Joback Method
cpg	891.75	J/mol×K	954.25	Joback Method
cpg	912.66	J/mol×K	990.04	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R345092&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