8«alpha»-Acetoxyelemol

Inchi: InChI=1S/C17H28O3/c1-8-17(7)10-15(20-12(4)18)14(16(5,6)19)9-13(17)11(2)3/h8,13-15
InchiKey: OVOINWQJBHVFGP-LSSORACZSA-N
Formula: C17H28O3
SMILES: C=CC1(C)CC(OC(C)=O)C(C(C)(C)O)CC1C(=C)C
Mol. weight [g/mol]: 280.40

Physical Properties

Property code	Value	Unit	Source
hfus	24.13	kJ/mol	Joback Method
logp	3.484		Crippen Method
mcvol	244.240	ml/mol	McGowan Method
rinpol	1788.00		NIST Webbook
rinpol	1775.00		NIST Webbook
rinpol	1779.00		NIST Webbook
rinpol	1781.00		NIST Webbook
rinpol	1782.00		NIST Webbook
rinpol	1789.00		NIST Webbook
rinpol	1788.00		NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	756.93	J/mol×K	752.62	Joback Method
cpg	775.57	J/mol×K	786.28	Joback Method
cpg	793.38	J/mol×K	819.93	Joback Method
cpg	810.47	J/mol×K	853.59	Joback Method
cpg	826.95	J/mol×K	887.25	Joback Method
cpg	842.93	J/mol×K	920.90	Joback Method
cpg	858.52	J/mol×K	954.56	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R613820&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	

Legend

cpg:	Ideal gas heat capacity
hfus:	Enthalpy of fusion at standard conditions
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices