7-Acetoxyelema-1,3-dien-8-ol

Inchi: InChI=1S/C17H26O2/c1-8-16(7)9-10-17(13(4)5,19-14(6)18)11-15(16)12(2)3/h8-10,13,15
InchiKey: ZCJSUCGQEIWWHR-IXDOHACOSA-N
Formula: C17H26O2
SMILES: C=CC1(C)C=CC(OC(C)=O)(C(C)C)CC1C(=C)C
Mol. weight [g/mol]: 262.39

Physical Properties

Property code	Value	Unit	Source
gf	51.04	kJ/mol	Joback Method
hf	-301.32	kJ/mol	Joback Method
hfus	17.78	kJ/mol	Joback Method
hvap	58.75	kJ/mol	Joback Method
log10ws	-4.64		Crippen Method
logp	4.289		Crippen Method
mcvol	234.070	ml/mol	McGowan Method
pc	1676.91	kPa	Joback Method
rinpol	1793.00		NIST Webbook
tb	667.30	K	Joback Method
tc	882.68	K	Joback Method
tf	368.49	K	Joback Method
vc	0.881	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	653.23	J/mol×K	667.30	Joback Method
cpg	673.74	J/mol×K	703.20	Joback Method
cpg	693.39	J/mol×K	739.09	Joback Method
cpg	712.38	J/mol×K	774.99	Joback Method
cpg	730.91	J/mol×K	810.89	Joback Method
cpg	749.18	J/mol×K	846.78	Joback Method
cpg	767.39	J/mol×K	882.68	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R281606&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume