3-Acetoxygermacra-1(10),5-dien-4-ol

Inchi: InChI=1S/C17H28O3/c1-12(2)15-8-6-13(3)7-9-16(20-14(4)18)17(5,19)11-10-15/h7,10-12
InchiKey: OWKZNKYCLMOXMD-HBQBMZAGSA-N
Formula: C17H28O3
SMILES: CC(=O)OC1CC=C(C)CCC(C(C)C)C=CC1(C)O
Mol. weight [g/mol]: 280.40

Physical Properties

Property code	Value	Unit	Source
gf	-275.49	kJ/mol	Joback Method
hf	-688.19	kJ/mol	Joback Method
hfus	24.47	kJ/mol	Joback Method
hvap	79.48	kJ/mol	Joback Method
log10ws	-4.41		Crippen Method
logp	3.628		Crippen Method
mcvol	244.240	ml/mol	McGowan Method
pc	1790.91	kPa	Joback Method
rinpol	1902.00		NIST Webbook
rinpol	1902.00		NIST Webbook
tb	787.22	K	Joback Method
tc	998.79	K	Joback Method
tf	422.09	K	Joback Method
vc	0.893	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	767.26	J/mol×K	787.22	Joback Method
cpg	786.67	J/mol×K	822.48	Joback Method
cpg	805.06	J/mol×K	857.74	Joback Method
cpg	822.50	J/mol×K	893.00	Joback Method
cpg	839.06	J/mol×K	928.26	Joback Method
cpg	854.81	J/mol×K	963.52	Joback Method
cpg	869.80	J/mol×K	998.79	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=R290190&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