(E, E)-5-Hydroxy-3,7,11-trimethyldodeca-2,6,10-trien-1 acetate

Inchi: InChI=1S/C17H28O3/c1-13(2)7-6-8-14(3)11-17(19)12-15(4)9-10-20-16(5)18/h7,9,11,17,1

InchiKey: WYRDKICJTLYOPH-SROZLARBSA-N

Formula: C17H28O3

SMILES: CC(=O)OCC=C(C)CC(O)C=C(C)CCC=C(C)C

Mol. weight [g/mol]: 280.40

Physical Properties

Property code	Value	Unit	Source
gf	-65.91	kJ/mol	Joback Method
hf	-474.23	kJ/mol	Joback Method
hfus	39.81	kJ/mol	Joback Method
hvap	79.00	kJ/mol	Joback Method
log10ws	-4.74		Crippen Method
logp	3.940		Crippen Method
mcvol	250.800	ml/mol	McGowan Method
pc	1558.58	kPa	Joback Method
rinpol	1959.00		NIST Webbook
rinpol	1959.00		NIST Webbook
tb	768.51	K	Joback Method
tc	956.99	K	Joback Method
tf	342.21	K	Joback Method
vc	0.968	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	733.92	J/mol×K	768.51	Joback Method
cpg	749.13	J/mol×K	799.92	Joback Method
cpg	763.58	J/mol×K	831.34	Joback Method
cpg	777.34	J/mol×K	862.75	Joback Method
cpg	790.45	J/mol×K	894.17	Joback Method
cpg	802.96	J/mol×K	925.58	Joback Method
cpg	814.93	J/mol×K	956.99	Joback Method

Sources

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=R227380&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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