3-Acetoxyamorpha-4,7(11)-dien-8-one

Inchi: InChI=1S/C17H24O3/c1-9(2)17-14-6-11(4)16(20-12(5)18)8-13(14)10(3)7-15(17)19/h6,10
InchiKey: HIEJMYXUMUNVKS-GDKBLKOGSA-N
Formula: C17H24O3
SMILES: CC(=O)OC1CC2C(C)CC(=O)C(=C(C)C)C2C=C1C
Mol. weight [g/mol]: 276.37

Physical Properties

Property code	Value	Unit	Source
gf	-149.33	kJ/mol	Joback Method
hf	-583.88	kJ/mol	Joback Method
hfus	31.94	kJ/mol	Joback Method
hvap	68.56	kJ/mol	Joback Method
log10ws	-3.96		Crippen Method
logp	3.446		Crippen Method
mcvol	229.080	ml/mol	McGowan Method
pc	1707.53	kPa	Joback Method
rinpol	1965.00		NIST Webbook
rinpol	1965.00		NIST Webbook
tb	764.35	K	Joback Method
tc	990.00	K	Joback Method
tf	444.73	K	Joback Method
vc	0.869	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	713.29	J/mol×K	764.35	Joback Method
cpg	733.24	J/mol×K	801.96	Joback Method
cpg	751.73	J/mol×K	839.57	Joback Method
cpg	768.77	J/mol×K	877.17	Joback Method
cpg	784.36	J/mol×K	914.78	Joback Method
cpg	798.50	J/mol×K	952.39	Joback Method
cpg	811.20	J/mol×K	990.00	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R226956&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