4-Hydroxy-2-isopropenyl-5-methylhex-5-enyl acetate, epimer

Inchi: InChI=1S/C12H20O3/c1-8(2)11(7-15-10(5)13)6-12(14)9(3)4/h11-12,14H,1,3,6-7H2,2,4-5

InchiKey: WZDDZSJLPOFSIZ-UHFFFAOYSA-N

Formula: C12H20O3

SMILES: C=C(C)C(O)CC(COC(C)=O)C(=C)C

Mol. weight [g/mol]: 212.29

Physical Properties

Property code	Value	Unit	Source
gf	-166.88	kJ/mol	Joback Method
hf	-467.32	kJ/mol	Joback Method
hfus	21.48	kJ/mol	Joback Method
hvap	66.19	kJ/mol	Joback Method
log10ws	-2.55		Crippen Method
logp	2.069		Crippen Method
mcvol	184.650	ml/mol	McGowan Method
pc	2220.80	kPa	Joback Method
rinpol	1407.00		NIST Webbook
rinpol	1407.00		NIST Webbook
ripol	2172.00		NIST Webbook
ripol	2172.00		NIST Webbook
tb	634.67	K	Joback Method
tc	814.83	K	Joback Method
tf	296.54	K	Joback Method
vc	0.703	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	486.19	J/mol×K	634.67	Joback Method
cpg	499.46	J/mol×K	664.70	Joback Method
cpg	512.08	J/mol×K	694.72	Joback Method
cpg	524.07	J/mol×K	724.75	Joback Method
cpg	535.46	J/mol×K	754.78	Joback Method
cpg	546.26	J/mol×K	784.80	Joback Method

cpg	556.49	J/mol×K	814.83	Joback Method

Sources

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=R232496&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume