(E)-5-Hydroxy-2-isopropenyl-5-methylhex-3-enyl acetate

Inchi: InChI=1S/C12H20O3/c1-9(2)11(8-15-10(3)13)6-7-12(4,5)14/h6-7,11,14H,1,8H2,2-5H3/b7
InchiKey: VJCYZSSRCAPSRC-VOTSOKGWSA-N
Formula: C12H20O3
SMILES: C=C(C)C(C=CC(C)(C)O)COC(C)=O
Mol. weight [g/mol]: 212.29

Physical Properties

Property code	Value	Unit	Source
gf	-160.67	kJ/mol	Joback Method
hf	-469.21	kJ/mol	Joback Method
hfus	20.39	kJ/mol	Joback Method
hvap	65.83	kJ/mol	Joback Method
log10ws	-2.55		Crippen Method
logp	2.069		Crippen Method
mcvol	184.650	ml/mol	McGowan Method
pc	2254.67	kPa	Joback Method
rinpol	1351.00		NIST Webbook
ripol	2022.00		NIST Webbook
ripol	2022.00		NIST Webbook
tb	639.48	K	Joback Method
tc	825.98	K	Joback Method
tf	324.60	K	Joback Method
vc	0.696	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	489.80	J/mol×K	639.48	Joback Method
cpg	503.16	J/mol×K	670.56	Joback Method
cpg	515.78	J/mol×K	701.65	Joback Method
cpg	527.71	J/mol×K	732.73	Joback Method
cpg	538.99	J/mol×K	763.81	Joback Method
cpg	549.64	J/mol×K	794.90	Joback Method
cpg	559.72	J/mol×K	825.98	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R232649&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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