(E)-5-Hydroxy-2-isopropenyl-5-methyl-hex-3-enyl isobutyrate

Inchi: InChI=1S/C14H24O3/c1-10(2)12(7-8-14(5,6)16)9-17-13(15)11(3)4/h7-8,11-12,16H,1,9H2

InchiKey: RGOXNJSZBDJLHQ-BQYQJAHWSA-N

Formula: C14H24O3

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

Mol. weight [g/mol]: 240.34

Physical Properties

Property code	Value	Unit	Source
gf	-146.27	kJ/mol	Joback Method
hf	-515.77	kJ/mol	Joback Method
hfus	22.04	kJ/mol	Joback Method
hvap	69.89	kJ/mol	Joback Method
log10ws	-3.14		Crippen Method
logp	2.705		Crippen Method
mcvol	212.830	ml/mol	McGowan Method
pc	1906.90	kPa	Joback Method
rinpol	1488.00		NIST Webbook
ripol	2086.00		NIST Webbook
tb	684.80	K	Joback Method
tc	871.40	K	Joback Method
tf	332.14	K	Joback Method
vc	0.801	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	594.65	J/mol×K	684.80	Joback Method
cpg	609.24	J/mol×K	715.90	Joback Method
cpg	623.03	J/mol×K	747.00	Joback Method
cpg	636.07	J/mol×K	778.10	Joback Method
cpg	648.39	J/mol×K	809.20	Joback Method
cpg	660.05	J/mol×K	840.30	Joback Method
cpg	671.07	J/mol×K	871.40	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=R232654&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume