4-Hydroxy-2-isopropenyl-5-methylhex-5-enyl isobutyrate

Inchi: InChI=1S/C14H24O3/c1-9(2)12(7-13(15)10(3)4)8-17-14(16)11(5)6/h11-13,15H,1,3,7-8H2

InchiKey: JRPNUBRUVFUHGJ-UHFFFAOYSA-N

Formula: C14H24O3

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

Mol. weight [g/mol]: 240.34

Physical Properties

Property code	Value	Unit	Source
gf	-152.48	kJ/mol	Joback Method
hf	-513.88	kJ/mol	Joback Method
hfus	23.14	kJ/mol	Joback Method
hvap	70.25	kJ/mol	Joback Method
log10ws	-3.14		Crippen Method
logp	2.705		Crippen Method
mcvol	212.830	ml/mol	McGowan Method
pc	1880.53	kPa	Joback Method
rinpol	1539.00		NIST Webbook
ripol	2229.00		NIST Webbook
tb	679.99	K	Joback Method
tc	860.92	K	Joback Method
tf	304.08	K	Joback Method
vc	0.808	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	591.23	J/mol×K	679.99	Joback Method
cpg	605.81	J/mol×K	710.14	Joback Method
cpg	619.66	J/mol×K	740.30	Joback Method
cpg	632.79	J/mol×K	770.45	Joback Method
cpg	645.24	J/mol×K	800.61	Joback Method
cpg	657.02	J/mol×K	830.76	Joback Method
cpg	668.16	J/mol×K	860.92	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=R232505&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