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

Inchi: InChI=1S/C15H26O3/c1-11(2)9-14(16)18-10-13(12(3)4)7-8-15(5,6)17/h7-8,11,13,17H,3,9

InchiKey: GEUJVWYWFCONDI-BQYQJAHWSA-N

Formula: C15H26O3

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

Mol. weight [g/mol]: 254.37

Physical Properties

Property code	Value	Unit	Source
gf	-137.85	kJ/mol	Joback Method
hf	-536.41	kJ/mol	Joback Method
hfus	24.63	kJ/mol	Joback Method
hvap	72.12	kJ/mol	Joback Method
log10ws	-3.56		Crippen Method
logp	3.095		Crippen Method
mcvol	226.920	ml/mol	McGowan Method
pc	1756.54	kPa	Joback Method
rinpol	1577.00		NIST Webbook
ripol	2179.00		NIST Webbook
ripol	2179.00		NIST Webbook
tb	707.68	K	Joback Method
tc	893.36	K	Joback Method
tf	343.41	K	Joback Method
vc	0.858	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	648.76	J/mol×K	707.68	Joback Method
cpg	663.77	J/mol×K	738.63	Joback Method
cpg	677.97	J/mol×K	769.57	Joback Method
cpg	691.41	J/mol×K	800.52	Joback Method
cpg	704.11	J/mol×K	831.47	Joback Method
cpg	716.14	J/mol×K	862.41	Joback Method
cpg	727.54	J/mol×K	893.36	Joback Method

Sources

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=R232634&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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