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

Inchi: InChI=1S/C15H26O3/c1-7-12(6)15(17)18-9-13(10(2)3)8-14(16)11(4)5/h12-14,16H,2,4,7-

InchiKey: YQYGOUBLFZCTSE-UHFFFAOYSA-N

Formula: C15H26O3

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

Mol. weight [g/mol]: 254.37

Physical Properties

Property code	Value	Unit	Source
gf	-144.06	kJ/mol	Joback Method
hf	-534.52	kJ/mol	Joback Method
hfus	25.73	kJ/mol	Joback Method
hvap	72.47	kJ/mol	Joback Method
log10ws	-3.56		Crippen Method
logp	3.095		Crippen Method
mcvol	226.920	ml/mol	McGowan Method
pc	1733.22	kPa	Joback Method
rinpol	1628.00		NIST Webbook
ripol	2309.00		NIST Webbook
tb	702.87	K	Joback Method
tc	883.34	K	Joback Method
tf	315.35	K	Joback Method
vc	0.865	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	645.48	J/mol×K	702.87	Joback Method
cpg	660.53	J/mol×K	732.95	Joback Method
cpg	674.82	J/mol×K	763.03	Joback Method
cpg	688.36	J/mol×K	793.11	Joback Method
cpg	701.19	J/mol×K	823.18	Joback Method
cpg	713.33	J/mol×K	853.26	Joback Method
cpg	724.80	J/mol×K	883.34	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=R232476&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

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