2-hydroxy-2-methyl-3-butenyl Angelate

Inchi: InChI=1S/C10H16O3/c1-5-8(3)9(11)13-7-10(4,12)6-2/h5-6,12H,2,7H2,1,3-4H3/b8-5-
InchiKey: QQSQGJPTALGCLH-YVMONPNESA-N
Formula: C10H16O3
SMILES: C=CC(C)(O)COC(=O)C(C)=CC
Mol. weight [g/mol]: 184.23

Physical Properties

Property code	Value	Unit	Source
gf	-175.07	kJ/mol	Joback Method
hf	-422.65	kJ/mol	Joback Method
hfus	18.73	kJ/mol	Joback Method
hvap	61.76	kJ/mol	Joback Method
log10ws	-1.95		Crippen Method
logp	1.433		Crippen Method
mcvol	156.470	ml/mol	McGowan Method
pc	2707.03	kPa	Joback Method
rinpol	1247.00		NIST Webbook
tb	594.16	K	Joback Method
tc	781.09	K	Joback Method
tf	317.06	K	Joback Method
vc	0.590	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	390.67	J/mol×K	594.16	Joback Method
cpg	402.54	J/mol×K	625.31	Joback Method
cpg	413.75	J/mol×K	656.47	Joback Method
cpg	424.34	J/mol×K	687.62	Joback Method
cpg	434.33	J/mol×K	718.78	Joback Method
cpg	443.76	J/mol×K	749.93	Joback Method
cpg	452.68	J/mol×K	781.09	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R438416&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume