(E)-3-Hydroxyfarnesa-1,6,10-trien-9-yl 2-methylbutyrate

Inchi: InChI=1S/C20H34O3/c1-8-17(6)19(21)23-18(13-15(3)4)14-16(5)11-10-12-20(7,22)9-2/h9
InchiKey: GPAYZXDFRBRXPA-LFIBNONCSA-N
Formula: C20H34O3
SMILES: C=CC(C)(O)CCC=C(C)CC(C=C(C)C)OC(=O)C(C)CC
Mol. weight [g/mol]: 322.48

Physical Properties

Property code	Value	Unit	Source
gf	-24.08	kJ/mol	Joback Method
hf	-532.18	kJ/mol	Joback Method
hfus	36.48	kJ/mol	Joback Method
hvap	83.28	kJ/mol	Joback Method
log10ws	-5.86		Crippen Method
logp	4.964		Crippen Method
mcvol	293.070	ml/mol	McGowan Method
pc	1267.35	kPa	Joback Method
rinpol	1969.00		NIST Webbook
rinpol	1969.00		NIST Webbook
ripol	2562.00		NIST Webbook
tb	826.12	K	Joback Method
tc	1019.49	K	Joback Method
tf	380.72	K	Joback Method
vc	1.119	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	909.31	J/mol×K	826.12	Joback Method
cpg	925.90	J/mol×K	858.35	Joback Method
cpg	941.65	J/mol×K	890.58	Joback Method
cpg	956.60	J/mol×K	922.81	Joback Method
cpg	970.85	J/mol×K	955.03	Joback Method
cpg	984.45	J/mol×K	987.26	Joback Method
cpg	997.48	J/mol×K	1019.49	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R232609&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

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