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

Other names: 3-Hydroxy-3,7,11-trimethyldodeca-1,6(E),10-trien-9-yl isobutyrate
Inchi: InChI=1S/C19H32O3/c1-8-19(7,21)11-9-10-16(6)13-17(12-14(2)3)22-18(20)15(4)5/h8,10
InchiKey: FSIHKFFUYHQELZ-MHWRWJLKSA-N
Formula: C19H32O3
SMILES: C=CC(C)(O)CCC=C(C)CC(C=C(C)C)OC(=O)C(C)C
Mol. weight [g/mol]: 308.46

Physical Properties

Property code	Value	Unit	Source
gf	-32.50	kJ/mol	Joback Method
hf	-511.54	kJ/mol	Joback Method
hfus	33.88	kJ/mol	Joback Method
hvap	81.06	kJ/mol	Joback Method
log10ws	-5.44		Crippen Method
logp	4.574		Crippen Method
mcvol	278.980	ml/mol	McGowan Method
pc	1358.63	kPa	Joback Method
rinpol	1881.00		NIST Webbook
rinpol	1881.00		NIST Webbook
rinpol	1882.00		NIST Webbook
ripol	2475.00		NIST Webbook
ripol	2485.00		NIST Webbook
ripol	2475.00		NIST Webbook
tb	803.24	K	Joback Method
tc	995.43	K	Joback Method
tf	369.45	K	Joback Method
vc	1.062	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	850.50	J/mol×K	803.24	Joback Method
cpg	866.69	J/mol×K	835.27	Joback Method
cpg	882.03	J/mol×K	867.30	Joback Method

cpg	896.60	J/mol×K	899.34	Joback Method
cpg	910.46	J/mol×K	931.37	Joback Method
cpg	923.67	J/mol×K	963.40	Joback Method
cpg	936.31	J/mol×K	995.43	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R232614&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