3-Hydroxy-3,7,11-trimethyldodeca-1,6(E),10-trien-9 propanoate

Inchi: InChI=1S/C18H30O3/c1-7-17(19)21-16(12-14(3)4)13-15(5)10-9-11-18(6,20)8-2/h8,10,12
InchiKey: WYWLOZXPFDNZML-XNTDXEJSSA-N
Formula: C18H30O3
SMILES: C=CC(C)(O)CCC=C(C)CC(C=C(C)C)OC(=O)CC
Mol. weight [g/mol]: 294.43

Physical Properties

Property code	Value	Unit	Source
gf	-38.48	kJ/mol	Joback Method
hf	-485.62	kJ/mol	Joback Method
hfus	34.82	kJ/mol	Joback Method
hvap	79.22	kJ/mol	Joback Method
log10ws	-5.27		Crippen Method
logp	4.328		Crippen Method
mcvol	264.890	ml/mol	McGowan Method
pc	1451.25	kPa	Joback Method
rinpol	1757.00		NIST Webbook
rinpol	1757.00		NIST Webbook
ripol	2378.00		NIST Webbook
ripol	2378.00		NIST Webbook
tb	780.80	K	Joback Method
tc	970.56	K	Joback Method
tf	373.18	K	Joback Method
vc	1.012	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	792.09	J/mol×K	780.80	Joback Method
cpg	807.74	J/mol×K	812.43	Joback Method
cpg	822.57	J/mol×K	844.05	Joback Method
cpg	836.65	J/mol×K	875.68	Joback Method
cpg	850.04	J/mol×K	907.31	Joback Method
cpg	862.81	J/mol×K	938.93	Joback Method

cpg	875.02	J/mol×K	970.56	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R420267&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume