(+)-«gamma»-Tocopherol, O-acetyl-

Inchi: InChI=1S/C30H50O3/c1-21(2)12-9-13-22(3)14-10-15-23(4)16-11-18-30(8)19-17-27-20-2
InchiKey: FOYKKGHVWRFIBD-UHFFFAOYSA-N
Formula: C30H50O3
SMILES: CC(=O)Oc1cc2c(c(C)c1C)OC(C)(CCCC(C)CCCC(C)CCCC(C)C)CC2
Mol. weight [g/mol]: 458.72

Physical Properties

Property code	Value	Unit	Source
gf	-8.59	kJ/mol	Joback Method
hf	-782.64	kJ/mol	Joback Method
hfus	55.87	kJ/mol	Joback Method
hvap	98.73	kJ/mol	Joback Method
log10ws	-10.06		Crippen Method
logp	8.752		Crippen Method
mcvol	412.250	ml/mol	McGowan Method
pc	786.39	kPa	Joback Method
rinpol	3118.00		NIST Webbook
rinpol	3118.00		NIST Webbook
tb	1045.57	K	Joback Method
tc	1280.58	K	Joback Method
tf	596.41	K	Joback Method
vc	1.581	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1485.38	J/mol×K	1045.57	Joback Method
cpg	1511.89	J/mol×K	1084.74	Joback Method
cpg	1538.07	J/mol×K	1123.91	Joback Method
cpg	1564.14	J/mol×K	1163.08	Joback Method
cpg	1590.29	J/mol×K	1202.25	Joback Method
cpg	1616.73	J/mol×K	1241.42	Joback Method
cpg	1643.67	J/mol×K	1280.58	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U374723&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume