(+)-«alpha»-Tocopherol, O-pentafluoropropionyl-

Inchi: InChI=1S/C32H49F5O3/c1-20(2)12-9-13-21(3)14-10-15-22(4)16-11-18-30(8)19-17-26-25

InchiKey: ZWZMZLFSLHSUSY-UHFFFAOYSA-N

Formula: C32H49F5O3

SMILES: Cc1c(C)c2c(c(C)c1OC(=O)C(F)(F)C(F)(F)F)CCC(C)(CCCC(C)CCCC(C)CCCC(C)C)O2

Mol. weight [g/mol]: 576.72

Physical Properties

Property code	Value	Unit	Source
gf	-969.75	kJ/mol	Joback Method
hf	-1833.44	kJ/mol	Joback Method
hfus	61.24	kJ/mol	Joback Method
hvap	97.17	kJ/mol	Joback Method
log10ws	-11.93		Crippen Method
logp	10.238		Crippen Method
mcvol	449.280	ml/mol	McGowan Method
pc	637.69	kPa	Joback Method
rinpol	2924.00		NIST Webbook
tb	1086.20	K	Joback Method
tc	1344.08	K	Joback Method
tf	639.26	K	Joback Method
vc	1.762	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1653.33	J/mol×K	1086.20	Joback Method
cpg	1683.51	J/mol×K	1129.18	Joback Method
cpg	1713.99	J/mol×K	1172.16	Joback Method
cpg	1745.13	J/mol×K	1215.14	Joback Method
cpg	1777.26	J/mol×K	1258.12	Joback Method
cpg	1810.75	J/mol×K	1301.10	Joback Method
cpg	1845.93	J/mol×K	1344.08	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U374717&Units=SI

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