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

Inchi: InChI=1S/C31H49F3O3/c1-20(2)12-9-13-21(3)14-10-15-22(4)16-11-18-30(8)19-17-26-25
InchiKey: WYAUJGNEMXZKRS-UHFFFAOYSA-N
Formula: C31H49F3O3
SMILES: Cc1c(C)c2c(c(C)c1OC(=O)C(F)(F)F)CCC(C)(CCCC(C)CCCC(C)CCCC(C)C)O2
Mol. weight [g/mol]: 526.71

Physical Properties

Property code	Value	Unit	Source
gf	-591.39	kJ/mol	Joback Method
hf	-1411.83	kJ/mol	Joback Method
hfus	59.90	kJ/mol	Joback Method
hvap	97.88	kJ/mol	Joback Method
log10ws	-11.20		Crippen Method
logp	9.602		Crippen Method
mcvol	431.650	ml/mol	McGowan Method
pc	695.08	kPa	Joback Method
rinpol	2918.00		NIST Webbook
rinpol	2918.00		NIST Webbook
tb	1068.01	K	Joback Method
tc	1314.18	K	Joback Method
tf	624.39	K	Joback Method
vc	1.681	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1572.44	J/mol×K	1068.01	Joback Method
cpg	1600.48	J/mol×K	1109.04	Joback Method
cpg	1628.45	J/mol×K	1150.07	Joback Method
cpg	1656.62	J/mol×K	1191.09	Joback Method
cpg	1685.25	J/mol×K	1232.12	Joback Method
cpg	1714.61	J/mol×K	1273.15	Joback Method
cpg	1744.96	J/mol×K	1314.18	Joback Method

Sources

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=U374716&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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