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

Inchi: InChI=1S/C33H49F7O3/c1-20(2)12-9-13-21(3)14-10-15-22(4)16-11-18-30(8)19-17-26-25
InchiKey: XCBODWISQPHZDL-UHFFFAOYSA-N
Formula: C33H49F7O3
SMILES: Cc1c(C)c2c(c(C)c1OC(=O)C(F)(F)C(F)(F)C(F)(F)F)CCC(C)(CCCC(C)CCCC(C)CCCC(C)
Mol. weight [g/mol]: 626.73

Physical Properties

Property code	Value	Unit	Source
gf	-1348.11	kJ/mol	Joback Method
hf	-2255.05	kJ/mol	Joback Method
hfus	62.57	kJ/mol	Joback Method
hvap	96.47	kJ/mol	Joback Method
log10ws	-12.66		Crippen Method
logp	10.873		Crippen Method
mcvol	466.910	ml/mol	McGowan Method
pc	587.13	kPa	Joback Method
rinpol	2953.00		NIST Webbook
tb	1104.39	K	Joback Method
tc	1377.18	K	Joback Method
tf	654.13	K	Joback Method
vc	1.843	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1734.87	J/mol×K	1104.39	Joback Method
cpg	1767.93	J/mol×K	1149.85	Joback Method
cpg	1801.79	J/mol×K	1195.32	Joback Method
cpg	1836.94	J/mol×K	1240.78	Joback Method
cpg	1873.82	J/mol×K	1286.25	Joback Method
cpg	1912.93	J/mol×K	1331.71	Joback Method
cpg	1954.71	J/mol×K	1377.18	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U374718&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume