«beta»-Tocopherol, O-pentafluoropropionyl-

Inchi: InChI=1S/C31H47F5O3/c1-20(2)11-8-12-21(3)13-9-14-22(4)15-10-17-29(7)18-16-25-24(
InchiKey: BFYRGFPQIGMCAG-UHFFFAOYSA-N
Formula: C31H47F5O3
SMILES: Cc1cc(OC(=O)C(F)(F)C(F)(F)F)c(C)c2c1OC(C)(CCCC(C)CCCC(C)CCCC(C)C)CC2
Mol. weight [g/mol]: 562.70

Physical Properties

Property code	Value	Unit	Source
gf	-968.54	kJ/mol	Joback Method
hf	-1801.33	kJ/mol	Joback Method
hfus	59.04	kJ/mol	Joback Method
hvap	94.28	kJ/mol	Joback Method
log10ws	-11.45		Crippen Method
logp	9.929		Crippen Method
mcvol	435.190	ml/mol	McGowan Method
pc	675.00	kPa	Joback Method
rinpol	2817.00		NIST Webbook
tb	1058.34	K	Joback Method
tc	1304.19	K	Joback Method
tf	615.47	K	Joback Method
vc	1.706	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1584.04	J/mol×K	1058.34	Joback Method
cpg	1612.09	J/mol×K	1099.32	Joback Method
cpg	1640.30	J/mol×K	1140.29	Joback Method
cpg	1668.97	J/mol×K	1181.27	Joback Method
cpg	1698.41	J/mol×K	1222.24	Joback Method
cpg	1728.93	J/mol×K	1263.22	Joback Method
cpg	1760.84	J/mol×K	1304.19	Joback Method

Sources

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=U374740&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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