«delta»-Tocopherol, O-pentafluoropropionyl-

Inchi: InChI=1S/C30H45F5O3/c1-20(2)10-7-11-21(3)12-8-13-22(4)14-9-16-28(6)17-15-24-19-2
InchiKey: HHBPUONUQXMRJU-UHFFFAOYSA-N
Formula: C30H45F5O3
SMILES: Cc1cc(OC(=O)C(F)(F)C(F)(F)F)cc2c1OC(C)(CCCC(C)CCCC(C)CCCC(C)C)CC2
Mol. weight [g/mol]: 548.67

Physical Properties

Property code	Value	Unit	Source
gf	-967.33	kJ/mol	Joback Method
hf	-1769.22	kJ/mol	Joback Method
hfus	56.84	kJ/mol	Joback Method
hvap	91.39	kJ/mol	Joback Method
log10ws	-10.98		Crippen Method
logp	9.621		Crippen Method
mcvol	421.100	ml/mol	McGowan Method
pc	715.68	kPa	Joback Method
rinpol	2726.00		NIST Webbook
tb	1030.48	K	Joback Method
tc	1265.90	K	Joback Method
tf	591.68	K	Joback Method
vc	1.649	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1515.70	J/mol×K	1030.48	Joback Method
cpg	1541.89	J/mol×K	1069.72	Joback Method
cpg	1568.10	J/mol×K	1108.95	Joback Method
cpg	1594.62	J/mol×K	1148.19	Joback Method
cpg	1621.71	J/mol×K	1187.43	Joback Method
cpg	1649.66	J/mol×K	1226.66	Joback Method
cpg	1678.74	J/mol×K	1265.90	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=U374732&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

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