«delta»-Tocopherol, O-heptafluorobutyryl-

Inchi: InChI=1S/C31H45F7O3/c1-20(2)10-7-11-21(3)12-8-13-22(4)14-9-16-28(6)17-15-24-19-2
InchiKey: PMCAQIGNKZLLAE-UHFFFAOYSA-N
Formula: C31H45F7O3
SMILES: Cc1cc(OC(=O)C(F)(F)C(F)(F)C(F)(F)F)cc2c1OC(C)(CCCC(C)CCCC(C)CCCC(C)C)CC2
Mol. weight [g/mol]: 598.68

Physical Properties

Property code	Value	Unit	Source
gf	-1345.69	kJ/mol	Joback Method
hf	-2190.83	kJ/mol	Joback Method
hfus	58.17	kJ/mol	Joback Method
hvap	90.69	kJ/mol	Joback Method
log10ws	-11.71		Crippen Method
logp	10.256		Crippen Method
mcvol	438.730	ml/mol	McGowan Method
pc	655.78	kPa	Joback Method
rinpol	2755.00		NIST Webbook
tb	1048.67	K	Joback Method
tc	1294.42	K	Joback Method
tf	606.55	K	Joback Method
vc	1.730	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1595.68	J/mol×K	1048.67	Joback Method
cpg	1623.67	J/mol×K	1089.63	Joback Method
cpg	1652.01	J/mol×K	1130.59	Joback Method
cpg	1681.06	J/mol×K	1171.54	Joback Method
cpg	1711.16	J/mol×K	1212.50	Joback Method
cpg	1742.68	J/mol×K	1253.46	Joback Method
cpg	1775.97	J/mol×K	1294.42	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=U374733&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