«delta»-Tocopherol, O-trifluoroacetyl-

Inchi: InChI=1S/C29H45F3O3/c1-20(2)10-7-11-21(3)12-8-13-22(4)14-9-16-28(6)17-15-24-19-2
InchiKey: BOTDPLUNGSNVJI-UHFFFAOYSA-N
Formula: C29H45F3O3
SMILES: Cc1cc(OC(=O)C(F)(F)F)cc2c1OC(C)(CCCC(C)CCCC(C)CCCC(C)C)CC2
Mol. weight [g/mol]: 498.66

Physical Properties

Property code	Value	Unit	Source
gf	-588.97	kJ/mol	Joback Method
hf	-1347.61	kJ/mol	Joback Method
hfus	55.50	kJ/mol	Joback Method
hvap	92.10	kJ/mol	Joback Method
log10ws	-10.24		Crippen Method
logp	8.986		Crippen Method
mcvol	403.470	ml/mol	McGowan Method
pc	784.19	kPa	Joback Method
rinpol	2738.00		NIST Webbook
tb	1012.29	K	Joback Method
tc	1240.19	K	Joback Method
tf	576.81	K	Joback Method
vc	1.569	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1436.15	J/mol×K	1012.29	Joback Method
cpg	1461.07	J/mol×K	1050.27	Joback Method
cpg	1485.78	J/mol×K	1088.26	Joback Method
cpg	1510.49	J/mol×K	1126.24	Joback Method
cpg	1535.41	J/mol×K	1164.22	Joback Method
cpg	1560.77	J/mol×K	1202.20	Joback Method
cpg	1586.78	J/mol×K	1240.19	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=U374734&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