«beta»-Tocopherol, O-trifluoroacetyl-

Inchi: InChI=1S/C30H47F3O3/c1-20(2)11-8-12-21(3)13-9-14-22(4)15-10-17-29(7)18-16-25-24(
InchiKey: BXRREPKFSOBBEK-UHFFFAOYSA-N
Formula: C30H47F3O3
SMILES: Cc1cc(OC(=O)C(F)(F)F)c(C)c2c1OC(C)(CCCC(C)CCCC(C)CCCC(C)C)CC2
Mol. weight [g/mol]: 512.69

Physical Properties

Property code	Value	Unit	Source
gf	-590.18	kJ/mol	Joback Method
hf	-1379.72	kJ/mol	Joback Method
hfus	57.70	kJ/mol	Joback Method
hvap	94.99	kJ/mol	Joback Method
log10ws	-10.72		Crippen Method
logp	9.294		Crippen Method
mcvol	417.560	ml/mol	McGowan Method
pc	737.62	kPa	Joback Method
rinpol	2822.00		NIST Webbook
rinpol	2822.00		NIST Webbook
tb	1040.15	K	Joback Method
tc	1276.46	K	Joback Method
tf	600.60	K	Joback Method
vc	1.625	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1503.84	J/mol×K	1040.15	Joback Method
cpg	1530.23	J/mol×K	1079.54	Joback Method
cpg	1556.46	J/mol×K	1118.92	Joback Method
cpg	1582.79	J/mol×K	1158.31	Joback Method
cpg	1609.45	J/mol×K	1197.69	Joback Method
cpg	1636.69	J/mol×K	1237.08	Joback Method
cpg	1664.73	J/mol×K	1276.46	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=U374739&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