«delta»-Tocopherol, O-acetyl-

Inchi: InChI=1S/C29H48O3/c1-21(2)11-8-12-22(3)13-9-14-23(4)15-10-17-29(7)18-16-26-20-27
InchiKey: TZGGOZSKJGOUCF-UHFFFAOYSA-N
Formula: C29H48O3
SMILES: CC(=O)Oc1cc(C)c2c(c1)CCC(C)(CCCC(C)CCCC(C)CCCC(C)C)O2
Mol. weight [g/mol]: 444.69

Physical Properties

Property code	Value	Unit	Source
gf	-7.38	kJ/mol	Joback Method
hf	-750.53	kJ/mol	Joback Method
hfus	53.67	kJ/mol	Joback Method
hvap	95.85	kJ/mol	Joback Method
log10ws	-9.58		Crippen Method
logp	8.443		Crippen Method
mcvol	398.160	ml/mol	McGowan Method
pc	837.73	kPa	Joback Method
rinpol	3027.00		NIST Webbook
tb	1017.71	K	Joback Method
tc	1245.97	K	Joback Method
tf	572.62	K	Joback Method
vc	1.526	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1417.29	J/mol×K	1017.71	Joback Method
cpg	1442.63	J/mol×K	1055.75	Joback Method
cpg	1467.61	J/mol×K	1093.80	Joback Method
cpg	1492.42	J/mol×K	1131.84	Joback Method
cpg	1517.24	J/mol×K	1169.88	Joback Method
cpg	1542.27	J/mol×K	1207.93	Joback Method
cpg	1567.71	J/mol×K	1245.97	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=U374731&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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