

# (.+/-.)-«alpha»-Tocopherol acetate

<b>Other names:</b>	(+)-.alpha.-Tocopherol, O-acetyl- (+)-«alpha»-Tocopherol acetate (+)-Â«alphaÂ»-Tocopherol acetate 2,5,7,8-Tetramethyl-2-(4,8,12-trimethyltridecyl)-3,4-dihydro-2H-chromen-6-yl acetate 2H-1-Benzopyran-6-ol, 3,4-dihydro-2,5,7,8-tetramethyl-2-(4,8,12-trimethyltridecyl)- acetate acetate DL-.alpha.-tocopherol acetate Vitamin E acetate dl-«alpha»-Tocopheryl acetate dl-Â«alphaÂ»-Tocopheryl acetate
<b>Inchi:</b>	InChI=1S/C31H52O3/c1-21(2)13-10-14-22(3)15-11-16-23(4)17-12-19-31(9)20-18-28-26(
<b>InchiKey:</b>	ZAKOWWREFLAJOT-UHFFFAOYSA-N
<b>Formula:</b>	C31H52O3
<b>SMILES:</b>	CC(=O)Oc1c(C)c(C)c2c(c1C)CCC(C)(CCCC(C)CCCC(C)CCCC(C)C)O2
<b>Mol. weight [g/mol]:</b>	472.74
<b>CAS:</b>	7695-91-2

## Physical Properties

Property code	Value	Unit	Source
gf	-9.80	kJ/mol	Joback Method
hf	-814.75	kJ/mol	Joback Method
hfus	58.08	kJ/mol	Joback Method
hvap	101.62	kJ/mol	Joback Method
log10ws	-10.53		Crippen Method
logp	9.060		Crippen Method
mcvol	426.340	ml/mol	McGowan Method
pc	739.63	kPa	Joback Method
rinpol	3194.00		NIST Webbook
rinpol	3194.00		NIST Webbook
tb	1073.43	K	Joback Method
tc	1316.54	K	Joback Method
tf	620.20	K	Joback Method
vc	1.637	m3/kmol	Joback Method

# Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1554.28	J/molxK	1073.43	Joback Method
cpg	1582.10	J/molxK	1113.95	Joback Method
cpg	1609.65	J/molxK	1154.47	Joback Method
cpg	1637.13	J/molxK	1194.99	Joback Method
cpg	1664.77	J/molxK	1235.51	Joback Method
cpg	1692.78	J/molxK	1276.02	Joback Method
cpg	1721.40	J/molxK	1316.54	Joback Method

## Sources

NIST Webbook:	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C7695912&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C7695912&amp;Units=SI</a>
Crippen Method:	<a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</a>
Crippen Method:	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>
Solubility of Vitamin E Acetate in Supercritical Carbon Dioxide: Measurement and Correlation	<a href="https://www.doi.org/10.1021/acs.jced.7b00550">https://www.doi.org/10.1021/acs.jced.7b00550</a>
Solubility of Vitamin E Acetate in Supercritical Carbon Dioxide with Ethanol as Co-solvent:	<a href="https://www.doi.org/10.1021/acs.jced.8b00745">https://www.doi.org/10.1021/acs.jced.8b00745</a>
Joback Method:	<a href="https://en.wikipedia.org/wiki/Joback_method">https://en.wikipedia.org/wiki/Joback_method</a>
McGowan Method:	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>

## Legend

<b>cpg:</b>	Ideal gas heat capacity
<b>gf:</b>	Standard Gibbs free energy of formation
<b>hf:</b>	Enthalpy of formation at standard conditions
<b>hfus:</b>	Enthalpy of fusion at standard conditions
<b>hvap:</b>	Enthalpy of vaporization at standard conditions
<b>log10ws:</b>	Log10 of Water solubility in mol/l
<b>logp:</b>	Octanol/Water partition coefficient
<b>mcvol:</b>	McGowan's characteristic volume
<b>pc:</b>	Critical Pressure
<b>rinpol:</b>	Non-polar retention indices
<b>tb:</b>	Normal Boiling Point Temperature
<b>tc:</b>	Critical Temperature
<b>tf:</b>	Normal melting (fusion) point

**vc:** Critical Volume

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