

«alpha»-Tocopheryl acetate

Other names:	2H-1-Benzopyran-6-ol, 3,4-dihydro-2,5,7,8-tetramethyl-2-(4,8,12-trimethyltridecyl)-, acetate, Vitamin E acetate [2R-[2R*(4R*,8R*)]]- 6-Chroman-2-ol, 2,5,7,8-tetramethyl-2-(4,8,12-trimethyltridecyl)-, acetate, (+)- «alpha»-Tocopherol acetate (+)-«alpha»-Tocopherol acetate (+)-«alpha»-Tocopheryl acetate D-«alpha»-tocopherol acetate D-«alpha»-tocopheryl acetate Alfacol Combinal E Contopheron E-Ferol E-Toplex Ecofrol Econ Endo E Dompe Ephynal acetate Epsilon-M Erevit Evipherol Fertilvit Gevex Juvela Tocopherex Tocophrin Tofaxin Tokoferol acetate [2R-[2R*(4R*,8R*)]]-3,4-Dihydro-2,5,7,8-tetramethyl-2-(4,8,12-trimethyltridecyl)-2H-1-benzopyran-6-ol acetate Vitamin E acetate E-vicotrat Spondyvit (2R,4'R,8'R)-«alpha»-Tocopheryl acetate (R,R,R)-«alpha»-Tocopheryl acetate Copherol 1250 Covitol 1100 Covitol 1360 Tocopheryl acetate Vitamin E alpha acetate
Inchi:	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(10,11,12,13,14,15,16,17,18,19,20,21,22,23,24,25,26,27,28,29,30,31)/h1-3,5-8,10-12,14-16,18-20,22-24,26-28,30-31/t2,4,6,8,10,12,14,16,18,20,22,24,26,28,30,31
InchiKey:	ZAKOWWREFLAJOT-BVXAZASISA-N

Formula:	C31H52O3
SMILES:	CC(=O)Oc1c(C)c(C)c2c(c1C)CCC(C)(CCCC(C)CCCC(C)CCCC(C)C)O2
Mol. weight [g/mol]:	472.74
CAS:	58-95-7

Physical Properties

Property code	Value	Unit	Source
chl	-18535.60 ± 7.50	kJ/mol	NIST Webbook
gf	-9.80	kJ/mol	Joback Method
hf	-814.75	kJ/mol	Joback Method
hfl	-1094.80 ± 7.50	kJ/mol	NIST Webbook
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	3132.00		NIST Webbook
rinpol	3131.00		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	1664.77	J/mol×K	1235.51	Joback Method
cpg	1692.78	J/mol×K	1276.02	Joback Method
cpg	1554.28	J/mol×K	1073.43	Joback Method
cpg	1582.10	J/mol×K	1113.95	Joback Method
cpg	1609.65	J/mol×K	1154.47	Joback Method
cpg	1637.13	J/mol×K	1194.99	Joback Method
cpg	1721.40	J/mol×K	1316.54	Joback Method
cps	898.00	J/mol×K	293.75	NIST Webbook
hvapt	60.10 ± 1.30	kJ/mol	495.00	NIST Webbook

Sources

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=C58957&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

chl:	Standard liquid enthalpy of combustion
cpg:	Ideal gas heat capacity
cps:	Solid phase heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfl:	Liquid phase enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
hvapt:	Enthalpy of vaporization at a given temperature
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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