«alpha»-Tocopheryl acetate

Other names:

2H-1-Benzopyran-6-ol, 3,4-dihydro-2,5,7,8-tetramethyl-2-(4,8,12-trimethyltridecyl)-, acetate, [2R-[2R*(4R*,8R*)]]-
Vitamin E acetate
6-Chromanol, 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
Epsilan-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-benz
d-Vitamin E acetate
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 Ealpha 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(

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	3131.00		NIST Webbook
rinpol	3132.00		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