Phytonadione

Other names:	Vitamin K1
	1,4-Naphthalenedione, 2-methyl-3-(3,7,11,15-tetramethyl-2-hexadecenyl)-, [R-[R*,R*-(E)]]-
	«alpha»-Phylloquinone
	trans-Phylloquinone
	Aqua Mephyton
	Combinal K1
	K-Ject
	Kativ N
	Kephton
	Kinadion
	Konakion
	Mephyton
	Mono-Kay
	Monodion
	Phyllochinon
	Phylloquinone
	Phythyl-menadion
	Phytomenadione
	Phytylmenadione
	Synthex P
	Vitamin K1(20)
	1,4-Naphthalenedione, 2-methyl-3-(3,7,11,15-tetramethyl-2-hexadecenyl)-
	2-Methyl-3-(3,7,11,15-tetramethyl-2-hexadecenyl)-1,4-naphthalenedione
	2',3'-trans-Vitamin K1
	Antihemorrhagic vitamin
	2-Methyl-3-phytyl-1,4-naphthochinon
	1,4-Naphthoquinone, 2-methyl-3-phytyl-
	[R-[R*,R*-(E)]]-2-Methyl-3-(3-7,11,15-tetramethyl-2-hexadecenyl)-1,4-naphthalenedione
	[R-[R*,R*-(E)]]-2-Methyl-3-(3,7,11,15-tetramethyl-2-hexadecenyl)-1,4-napthalenedione
	2-Methyl-3-phytyl-1,4-naphthoquinone
	3-Phytylmenadione
	Aqua-Mephytin
	NSC 270681
Inchi:	InChI=1S/C31H46O2/c1-22(2)12-9-13-23(3)14-10-15-24(4)16-11-17-25(5)20-21-27-26(6
InchiKey:	MBWXNTAXLNYFJB-JHBCSKSVSA-N
Formula:	C31H46O2
SMILES:	CC(=CCC1=C(C)C(=O)c2ccccc2C1=O)CCCC(C)CCCC(C)CCCC(C)C
Mol. weight [g/mol]:	450.70
CAS:	84-80-0

Physical Properties

Property code	Value	Unit	Source
gf	199.15	kJ/mol	Joback Method
hf	-520.10	kJ/mol	Joback Method
hfus	52.45	kJ/mol	Joback Method
hvap	96.92	kJ/mol	Joback Method
log10ws	-10.46		Crippen Method
logp	9.158		Crippen Method
mcvol	407.570	ml/mol	McGowan Method
pc	801.15	kPa	Joback Method
rinpol	3287.00		NIST Webbook
tb	1103.50	K	Joback Method
tc	1351.22	K	Joback Method
tf	594.93	K	Joback Method
vc	1.577	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1455.83	J/mol×K	1103.50	Joback Method
cpg	1473.31	J/mol×K	1144.79	Joback Method
cpg	1489.01	J/mol×K	1186.07	Joback Method
cpg	1503.03	J/mol×K	1227.36	Joback Method
cpg	1515.49	J/mol×K	1268.65	Joback Method
cpg	1526.46	J/mol×K	1309.93	Joback Method
cpg	1536.05	J/mol×K	1351.22	Joback Method

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=C84800&Units=SI

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

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