

# Vitamin k1

<b>Other names:</b>	2-Methyl-3-phytyl-1,4-naphthoquinone 2-methyl-3-(3,7,11,15-tetramethylhexadec-2-enyl)-1,4-naphthoquinone
<b>Inchi:</b>	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)
<b>InchiKey:</b>	MBWXNTAXLNYFJB-LKUDQCMESA-N
<b>Formula:</b>	C31H46O2
<b>SMILES:</b>	CC(=CCC1=C(C)C(=O)c2ccccc2C1=O)CCCC(C)CCCC(C)CCCC(C)C
<b>Mol. weight [g/mol]:</b>	450.70
<b>CAS:</b>	81818-54-4

## 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
mvol	407.570	ml/mol	McGowan Method
pc	801.15	kPa	Joback Method
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/molxK	1103.50	Joback Method
cpg	1473.31	J/molxK	1144.79	Joback Method
cpg	1489.01	J/molxK	1186.07	Joback Method
cpg	1503.03	J/molxK	1227.36	Joback Method
cpg	1515.49	J/molxK	1268.65	Joback Method
cpg	1526.46	J/molxK	1309.93	Joback Method
cpg	1536.05	J/molxK	1351.22	Joback Method

# Sources

<b>McGowan Method:</b>	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C81818544&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C81818544&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307l">http://pubs.acs.org/doi/abs/10.1021/ci990307l</a>
<b>Crippen Method:</b>	<a href="https://www.cheméo.com/doc/models/crippen_log10ws">https://www.cheméo.com/doc/models/crippen_log10ws</a>
<b>Joback Method:</b>	<a href="https://en.wikipedia.org/wiki/Joback_method">https://en.wikipedia.org/wiki/Joback_method</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>tb:</b>	Normal Boiling Point Temperature
<b>tc:</b>	Critical Temperature
<b>tf:</b>	Normal melting (fusion) point
<b>vc:</b>	Critical Volume

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