

# Phytyl tetradecanoate

<b>Inchi:</b>	InChI=1S/C34H66O2/c1-7-8-9-10-11-12-13-14-15-16-17-27-34(35)36-29-28-33(6)26-20-
<b>InchiKey:</b>	QYGFRAWKWSAZOD-PJLLUWSFSA-N
<b>Formula:</b>	C34H66O2
<b>SMILES:</b>	CCCCCCCCCCCC(=O)OCC=C(C)CCCC(C)CCCC(C)CCCC(C)C
<b>Mol. weight [g/mol]:</b>	506.89

## Physical Properties

Property code	Value	Unit	Source
gf	65.83	kJ/mol	Joback Method
hf	-898.30	kJ/mol	Joback Method
hfus	74.93	kJ/mol	Joback Method
hvap	99.31	kJ/mol	Joback Method
log10ws	-12.05		Crippen Method
logp	11.616		Crippen Method
mvol	493.060	ml/mol	McGowan Method
pc	527.26	kPa	Joback Method
rinpol	3361.90		NIST Webbook
rinpol	3361.90		NIST Webbook
tb	1056.33	K	Joback Method
tc	1328.14	K	Joback Method
tf	481.06	K	Joback Method
vc	1.927	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1790.71	J/mol×K	1056.33	Joback Method
cpg	1819.32	J/mol×K	1101.63	Joback Method
cpg	1845.69	J/mol×K	1146.93	Joback Method
cpg	1870.04	J/mol×K	1192.24	Joback Method
cpg	1892.56	J/mol×K	1237.54	Joback Method
cpg	1913.49	J/mol×K	1282.84	Joback Method
cpg	1933.01	J/mol×K	1328.14	Joback Method

# Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=U413674&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U413674&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</a>
<b>Crippen Method:</b>	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.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>
<b>McGowan Method:</b>	<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>hvpap:</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>rinppl:</b>	Non-polar retention indices
<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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