Phytyl tetradecanoate

Inchi: 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-
InchiKey: QYGFRANKWSAZOD-PJJLUWSFSA-N
Formula: C34H66O2
SMILES: CCCCCCCCCCCCCC(=O)OCC=C(C)CCCC(C)CCCC(C)CCCC(C)C
Mol. weight [g/mol]: 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
mcvol	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	m3/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

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
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=U413674&Units=SI

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

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