Phytyl palmitate

Inchi: InChI=1S/C36H70O2/c1-7-8-9-10-11-12-13-14-15-16-17-18-19-29-36(37)38-31-30-35(6)
InchiKey: JDFCEOMVLWWUMP-WUZYOQQESA-N
Formula: C36H70O2
SMILES: CCCCCCCCCCCCCCCC(=O)OCC=C(C)CCCC(C)CCCC(C)CCCC(C)C
Mol. weight [g/mol]: 534.94

Physical Properties

Property code	Value	Unit	Source
gf	82.67	kJ/mol	Joback Method
hf	-939.58	kJ/mol	Joback Method
hfus	80.11	kJ/mol	Joback Method
hvap	103.76	kJ/mol	Joback Method
log10ws	-12.88		Crippen Method
logp	12.396		Crippen Method
mcvol	521.240	ml/mol	McGowan Method
pc	483.67	kPa	Joback Method
rinpol	3509.30		NIST Webbook
rinpol	3509.30		NIST Webbook
tb	1102.09	K	Joback Method
tc	1407.81	K	Joback Method
tf	503.60	K	Joback Method
vc	2.038	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1926.89	J/mol×K	1102.09	Joback Method
cpg	1958.18	J/mol×K	1153.04	Joback Method
cpg	1986.81	J/mol×K	1204.00	Joback Method
cpg	2013.10	J/mol×K	1254.95	Joback Method
cpg	2037.35	J/mol×K	1305.90	Joback Method
cpg	2059.90	J/mol×K	1356.86	Joback Method
cpg	2081.05	J/mol×K	1407.81	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=U413678&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