Phytyl dodecanoate

Inchi: InChI=1S/C32H62O2/c1-7-8-9-10-11-12-13-14-15-25-32(33)34-27-26-31(6)24-18-23-30(
InchiKey: AGWFXWWNJHQGIB-GKPLWNPISA-N
Formula: C32H62O2
SMILES: CCCCCCCCCCCC(=O)OCC=C(C)CCCC(C)CCCC(C)CCCC(C)C
Mol. weight [g/mol]: 478.83

Physical Properties

Property code	Value	Unit	Source
gf	48.99	kJ/mol	Joback Method
hf	-857.02	kJ/mol	Joback Method
hfus	69.75	kJ/mol	Joback Method
hvap	94.86	kJ/mol	Joback Method
log10ws	-11.21		Crippen Method
logp	10.836		Crippen Method
mcvol	464.880	ml/mol	McGowan Method
pc	577.02	kPa	Joback Method
rinpol	3160.70		NIST Webbook
rinpol	3160.70		NIST Webbook
tb	1010.57	K	Joback Method
tc	1255.38	K	Joback Method
tf	458.52	K	Joback Method
vc	1.815	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1655.69	J/mol×K	1010.57	Joback Method
cpg	1682.10	J/mol×K	1051.37	Joback Method
cpg	1706.62	J/mol×K	1092.17	Joback Method
cpg	1729.39	J/mol×K	1132.98	Joback Method
cpg	1750.56	J/mol×K	1173.78	Joback Method
cpg	1770.27	J/mol×K	1214.58	Joback Method
cpg	1788.66	J/mol×K	1255.38	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=U413673&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