Phytyl decanoate

Inchi: InChI=1S/C30H58O2/c1-7-8-9-10-11-12-13-23-30(31)32-25-24-29(6)22-16-21-28(5)20-1
InchiKey: VQNBYXCYEWSWMZ-RMLRFSFXSA-N
Formula: C30H58O2
SMILES: CCCCCCCCCC(=O)OCC=C(C)CCCC(C)CCCC(C)CCCC(C)C
Mol. weight [g/mol]: 450.78

Physical Properties

Property code	Value	Unit	Source
gf	32.15	kJ/mol	Joback Method
hf	-815.74	kJ/mol	Joback Method
hfus	64.57	kJ/mol	Joback Method
hvap	90.40	kJ/mol	Joback Method
log10ws	-10.37		Crippen Method
logp	10.056		Crippen Method
mcvol	436.700	ml/mol	McGowan Method
pc	634.16	kPa	Joback Method
rinpol	2956.90		NIST Webbook
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tb	964.81	K	Joback Method
tc	1188.51	K	Joback Method
tf	435.98	K	Joback Method
vc	1.702	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1522.05	J/mol×K	964.81	Joback Method
cpg	1546.68	J/mol×K	1002.09	Joback Method
cpg	1569.69	J/mol×K	1039.38	Joback Method
cpg	1591.18	J/mol×K	1076.66	Joback Method
cpg	1611.25	J/mol×K	1113.94	Joback Method
cpg	1630.02	J/mol×K	1151.23	Joback Method
cpg	1647.57	J/mol×K	1188.51	Joback Method

Sources

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=U413902&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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