Phytyl stearate

Inchi: InChI=1S/C38H74O2/c1-7-8-9-10-11-12-13-14-15-16-17-18-19-20-21-31-38(39)40-33-32
InchiKey: GPIMVSWDTKPEPH-BQNXFWFHSA-N
Formula: C38H74O2
SMILES: CCCCCCCCCCCCCCCCCC(=O)OCC=C(C)CCCC(C)CCCC(C)CCCC(C)C
Mol. weight [g/mol]: 562.99
CAS: 62172-54-7

Physical Properties

Property code	Value	Unit	Source
gf	99.51	kJ/mol	Joback Method
hf	-980.86	kJ/mol	Joback Method
hfus	85.29	kJ/mol	Joback Method
hvap	108.21	kJ/mol	Joback Method
log10ws	-13.72		Crippen Method
logp	13.177		Crippen Method
mcvol	549.420	ml/mol	McGowan Method
pc	445.27	kPa	Joback Method
rinpol	3751.60		NIST Webbook
rinpol	3751.60		NIST Webbook
tb	1147.85	K	Joback Method
tc	1495.61	K	Joback Method
tf	526.14	K	Joback Method
vc	2.151	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	2064.04	J/mol×K	1147.85	Joback Method
cpg	2098.61	J/mol×K	1205.81	Joback Method
cpg	2130.00	J/mol×K	1263.77	Joback Method
cpg	2158.72	J/mol×K	1321.73	Joback Method
cpg	2185.25	J/mol×K	1379.69	Joback Method
cpg	2210.10	J/mol×K	1437.65	Joback Method
cpg	2233.76	J/mol×K	1495.61	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=C62172547&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