Phytyl, 2-methylbutanoate

Inchi: InChI=1S/C25H48O2/c1-8-24(7)25(26)27-19-18-23(6)17-11-16-22(5)15-10-14-21(4)13-9
InchiKey: PNYWYUSUVPFANG-PTGBLXJZSA-N
Formula: C25H48O2
SMILES: CCC(C)C(=O)OCC=C(C)CCCC(C)CCCC(C)CCCC(C)C
Mol. weight [g/mol]: 380.65

Physical Properties

Property code	Value	Unit	Source
gf	-12.39	kJ/mol	Joback Method
hf	-717.82	kJ/mol	Joback Method
hfus	48.09	kJ/mol	Joback Method
hvap	78.89	kJ/mol	Joback Method
log10ws	-8.04		Crippen Method
logp	7.961		Crippen Method
mcvol	366.250	ml/mol	McGowan Method
pc	824.31	kPa	Joback Method
rinpol	2440.90		NIST Webbook
rinpol	2440.90		NIST Webbook
tb	849.97	K	Joback Method
tc	1041.82	K	Joback Method
tf	364.63	K	Joback Method
vc	1.417	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1196.41	J/mol×K	849.97	Joback Method
cpg	1218.06	J/mol×K	881.94	Joback Method
cpg	1238.50	J/mol×K	913.92	Joback Method
cpg	1257.78	J/mol×K	945.89	Joback Method
cpg	1275.96	J/mol×K	977.87	Joback Method
cpg	1293.09	J/mol×K	1009.84	Joback Method
cpg	1309.21	J/mol×K	1041.82	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U413677&Units=SI
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

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