Isophytol, acetate

Inchi: InChI=1S/C22H42O2/c1-8-22(7,24-21(6)23)17-11-16-20(5)15-10-14-19(4)13-9-12-18(2)3
InchiKey: GKWIQRXSJFOVGL-UHFFFAOYSA-N
Formula: C22H42O2
SMILES: C=CC(C)(CCCC(C)CCCC(C)CCCC(C)C)OC(C)=O
Mol. weight [g/mol]: 338.57

Physical Properties

Property code	Value	Unit	Source
gf	-16.20	kJ/mol	Joback Method
hf	-641.37	kJ/mol	Joback Method
hfus	36.26	kJ/mol	Joback Method
hvap	70.59	kJ/mol	Joback Method
log10ws	-7.13		Crippen Method
logp	6.933		Crippen Method
mcvol	323.980	ml/mol	McGowan Method
pc	977.17	kPa	Joback Method
rinpol	2064.00		NIST Webbook
rinpol	2064.00		NIST Webbook
tb	771.18	K	Joback Method
tc	954.22	K	Joback Method
tf	365.52	K	Joback Method
vc	1.244	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1006.89	J/mol×K	771.18	Joback Method
cpg	1027.43	J/mol×K	801.69	Joback Method
cpg	1046.88	J/mol×K	832.19	Joback Method
cpg	1065.29	J/mol×K	862.70	Joback Method
cpg	1082.69	J/mol×K	893.21	Joback Method
cpg	1099.14	J/mol×K	923.72	Joback Method
cpg	1114.69	J/mol×K	954.22	Joback Method
dvisc	0.0029770	Pa×s	365.52	Joback Method

dvisc	0.0008131	Pa×s	433.13	Joback Method
dvisc	0.0003153	Pa×s	500.74	Joback Method
dvisc	0.0001532	Pa×s	568.35	Joback Method
dvisc	0.0000867	Pa×s	635.96	Joback Method
dvisc	0.0000548	Pa×s	703.57	Joback Method
dvisc	0.0000375	Pa×s	771.18	Joback Method

Sources

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=U374862&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

cpg: Ideal gas heat capacity
dvisc: Dynamic viscosity
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