Phytol, acetate

Other names: Phytyl acetate
trans-phytyl acetate
Inchi: InChI=1S/C22H42O2/c1-18(2)10-7-11-19(3)12-8-13-20(4)14-9-15-21(5)16-17-24-22(6)23
InchiKey: JIGCTXHIECXYRJ-LTGZKZEYSA-N
Formula: C22H42O2
SMILES: CC(=O)OCC=C(C)CCCC(C)CCCC(C)CCCC(C)C
Mol. weight [g/mol]: 338.57

Physical Properties

Property code	Value	Unit	Source
gf	-35.21	kJ/mol	Joback Method
hf	-650.62	kJ/mol	Joback Method
hfus	43.85	kJ/mol	Joback Method
hvap	72.60	kJ/mol	Joback Method
log10ws	-7.02		Crippen Method
logp	6.935		Crippen Method
mcvol	323.980	ml/mol	McGowan Method
pc	974.73	kPa	Joback Method
rinpol	2218.00		NIST Webbook
rinpol	2222.00		NIST Webbook
rinpol	2223.00		NIST Webbook
rinpol	2223.00		NIST Webbook
rinpol	2223.00		NIST Webbook
rinpol	2219.00		NIST Webbook
rinpol	2222.00		NIST Webbook
rinpol	2218.00		NIST Webbook
rinpol	2225.00		NIST Webbook
ripol	2438.00		NIST Webbook
ripol	2439.00		NIST Webbook
ripol	2438.00		NIST Webbook
tb	781.77	K	Joback Method
tc	964.72	K	Joback Method
tf	345.82	K	Joback Method
vc	1.254	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1007.80	J/mol×K	781.77	Joback Method
cpg	1028.28	J/mol×K	812.26	Joback Method
cpg	1047.70	J/mol×K	842.75	Joback Method
cpg	1066.10	J/mol×K	873.25	Joback Method
cpg	1083.53	J/mol×K	903.74	Joback Method
cpg	1100.03	J/mol×K	934.23	Joback Method
cpg	1115.63	J/mol×K	964.72	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=U375014&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
ripol: Polar retention indices
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume