cis-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-PGMHBOJBSA-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
ripol	2492.00		NIST Webbook
ripol	2491.00		NIST Webbook
ripol	2491.00		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

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R308335&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume