(Z)-Farnesyl acetate

Inchi: InChI=1S/C17H28O2/c1-14(2)8-6-9-15(3)10-7-11-16(4)12-13-19-17(5)18/h8,10,12H,6-7,
InchiKey: ZGIGZINMAOQWLX-DELZMPIMSA-N
Formula: C17H28O2
SMILES: CC(=O)OCC=C(C)CCC=C(C)CCC=C(C)C
Mol. weight [g/mol]: 264.40

Physical Properties

Property code	Value	Unit	Source
gf	73.35	kJ/mol	Joback Method
hf	-316.72	kJ/mol	Joback Method
hfus	39.25	kJ/mol	Joback Method
hvap	62.71	kJ/mol	Joback Method
log10ws	-5.36		Crippen Method
logp	4.969		Crippen Method
mcvol	244.930	ml/mol	McGowan Method
pc	1442.44	kPa	Joback Method
rinpol	1817.00		NIST Webbook
ripol	2214.00		NIST Webbook
tb	676.77	K	Joback Method
tc	866.41	K	Joback Method
tf	296.39	K	Joback Method
vc	0.955	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	666.60	J/mol×K	676.77	Joback Method
cpg	684.20	J/mol×K	708.38	Joback Method
cpg	700.91	J/mol×K	739.98	Joback Method
cpg	716.78	J/mol×K	771.59	Joback Method
cpg	731.87	J/mol×K	803.19	Joback Method
cpg	746.22	J/mol×K	834.80	Joback Method
cpg	759.89	J/mol×K	866.41	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=R299231&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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