(Z,E)-Farnesyl acetate

Other names: (2Z, 6E)-Farnesyl acetate
cis-trans-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-NCZFFCEISA-N
Formula: C17H28O2
SMILES: CC(=O)OCC=C(C)CCC=C(C)CCC=C(C)C
Mol. weight [g/mol]: 264.40
CAS: 40266-29-3

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	1775.00		NIST Webbook
rinpol	1822.00		NIST Webbook
rinpol	1808.00		NIST Webbook
rinpol	1822.00		NIST Webbook
rinpol	1787.00		NIST Webbook
rinpol	1776.00		NIST Webbook
rinpol	1808.00		NIST Webbook
rinpol	1804.00		NIST Webbook
rinpol	1805.00		NIST Webbook
rinpol	1822.00		NIST Webbook
rinpol	1792.00		NIST Webbook
rinpol	1824.00		NIST Webbook
rinpol	1812.00		NIST Webbook
rinpol	1822.00		NIST Webbook
rinpol	1818.00		NIST Webbook
rinpol	1818.00		NIST Webbook
rinpol	1788.00		NIST Webbook
rinpol	1818.00		NIST Webbook

rinpol	1814.00		NIST Webbook
rinpol	1804.00		NIST Webbook
ripol	2225.00		NIST Webbook
ripol	2225.00		NIST Webbook
ripol	2241.00		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

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=C40266293&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

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