Farnesyl acetate

Other names:	Farnesol, acetate
	3,7,11-trimethyldodeca-2,6,10-trienyl 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-UHFFFAOYSA-N
Formula:	C17H28O2
SMILES:	CC(=O)OCC=C(C)CCC=C(C)CCC=C(C)C
Mol. weight [g/mol]:	264.40
CAS:	29548-30-9

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	1834.00		NIST Webbook
rinpol	1815.00		NIST Webbook
rinpol	1831.00		NIST Webbook
rinpol	1846.00		NIST Webbook
rinpol	1822.00		NIST Webbook
rinpol	1835.30		NIST Webbook
rinpol	1834.00		NIST Webbook
rinpol	1817.00		NIST Webbook
rinpol	1804.00		NIST Webbook
rinpol	1794.50		NIST Webbook
rinpol	1818.00		NIST Webbook
rinpol	1790.00		NIST Webbook
rinpol	1787.00		NIST Webbook
rinpol	1817.60		NIST Webbook
rinpol	1820.00		NIST Webbook
rinpol	1820.00		NIST Webbook
rinpol	1790.00		NIST Webbook
ripol	2271.00		NIST Webbook

ripol	2244.00		NIST Webbook
ripol	2222.00		NIST Webbook
ripol	2271.00		NIST Webbook
ripol	2271.00		NIST Webbook
ripol	2271.00		NIST Webbook
ripol	2271.00		NIST Webbook
ripol	2271.00		NIST Webbook
ripol	2271.00		NIST Webbook
ripol	2271.00		NIST Webbook
ripol	2269.00		NIST Webbook
ripol	2245.00		NIST Webbook
ripol	2262.00		NIST Webbook
ripol	2250.00		NIST Webbook
ripol	2225.00		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

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C29548309&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

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