

2,3-Dihydro farnesyl acetate

Inchi:	InChI=1S/C17H30O2/c1-14(2)8-6-9-15(3)10-7-11-16(4)12-13-19-17(5)18/h8,10,16H,6-7,
InchiKey:	IAKSWXAQVICMSZ-XNTDXEJSSA-N
Formula:	C17H30O2
SMILES:	CC(=O)OCCC(C)CCC=C(C)CCC=C(C)C
Mol. weight [g/mol]:	266.42
CAS:	58130-58-8

Physical Properties

Property code	Value	Unit	Source
gf	-0.76	kJ/mol	Joback Method
hf	-429.43	kJ/mol	Joback Method
hfus	36.83	kJ/mol	Joback Method
hvap	62.28	kJ/mol	Joback Method
log10ws	-5.27		Crippen Method
logp	5.049		Crippen Method
mcvol	249.230	ml/mol	McGowan Method
pc	1390.22	kPa	Joback Method
rinpol	1840.00		NIST Webbook
rinpol	1805.40		NIST Webbook
rinpol	1840.00		NIST Webbook
rinpol	1805.40		NIST Webbook
tb	672.29	K	Joback Method
tc	856.36	K	Joback Method
tf	300.43	K	Joback Method
vc	0.968	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	689.18	J/mol×K	672.29	Joback Method
cpg	707.31	J/mol×K	702.97	Joback Method
cpg	724.55	J/mol×K	733.65	Joback Method
cpg	740.94	J/mol×K	764.33	Joback Method
cpg	756.52	J/mol×K	795.01	Joback Method

cpg	771.33	J/mol×K	825.69	Joback Method
cpg	785.40	J/mol×K	856.36	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=C58130588&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
hvac:	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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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