1-Hexen-3-ol, acetate

Other names: 1-propylallyl acetate
Inchi: InChI=1S/C8H14O2/c1-4-6-8(5-2)10-7(3)9/h5,8H,2,4,6H2,1,3H3
InchiKey: XCAHGFCKEWDQJK-UHFFFAOYSA-N
Formula: C8H14O2
SMILES: C=CC(CCC)OC(C)=O
Mol. weight [g/mol]: 142.20
CAS: 35926-04-6

Physical Properties

Property code	Value	Unit	Source
gf	-132.04	kJ/mol	Joback Method
hf	-333.10	kJ/mol	Joback Method
hfus	14.46	kJ/mol	Joback Method
hvap	41.50	kJ/mol	Joback Method
log10ws	-2.00		Crippen Method
logp	1.904		Crippen Method
mcvol	126.720	ml/mol	McGowan Method
pc	2799.47	kPa	Joback Method
rinpol	897.00		NIST Webbook
rinpol	897.00		NIST Webbook
tb	454.97	K	Joback Method
tc	637.48	K	Joback Method
tf	235.32	K	Joback Method
vc	0.482	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	263.19	J/mol×K	454.97	Joback Method
cpg	318.44	J/mol×K	607.06	Joback Method
cpg	308.30	J/mol×K	576.64	Joback Method
cpg	297.72	J/mol×K	546.22	Joback Method
cpg	286.67	J/mol×K	515.81	Joback Method
cpg	275.17	J/mol×K	485.39	Joback Method

cpg	328.12	J/mol×K	637.48	Joback Method
dvisc	0.0002428	Pa×s	454.97	Joback Method
dvisc	0.0003181	Pa×s	418.36	Joback Method
dvisc	0.0004389	Pa×s	381.75	Joback Method
dvisc	0.0006484	Pa×s	345.14	Joback Method
dvisc	0.0010509	Pa×s	308.54	Joback Method
dvisc	0.0019397	Pa×s	271.93	Joback Method
dvisc	0.0043324	Pa×s	235.32	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=C35926046&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
dvisc:	Dynamic viscosity
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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