4-Hepten-2-ol, (Z)-, acetate

Other names: (Z)-4-Hepten-2-yl, acetate
Inchi: InChI=1S/C9H16O2/c1-4-5-6-7-8(2)11-9(3)10/h5-6,8H,4,7H2,1-3H3/b6-5-
InchiKey: QJMRCUOWTUQXIQ-WAYWQWQTSA-N
Formula: C9H16O2
SMILES: CCC=CCC(C)OC(C)=O
Mol. weight [g/mol]: 156.22

Physical Properties

Property code	Value	Unit	Source
gf	-131.24	kJ/mol	Joback Method
hf	-361.95	kJ/mol	Joback Method
hfus	18.53	kJ/mol	Joback Method
hvap	44.35	kJ/mol	Joback Method
log10ws	-2.42		Crippen Method
logp	2.294		Crippen Method
mcvol	140.810	ml/mol	McGowan Method
pc	2561.10	kPa	Joback Method
rinpol	1024.00		NIST Webbook
rinpol	1022.00		NIST Webbook
rinpol	1022.00		NIST Webbook
rinpol	1023.00		NIST Webbook
rinpol	1023.00		NIST Webbook
tb	485.33	K	Joback Method
tc	670.77	K	Joback Method
tf	243.27	K	Joback Method
vc	0.537	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	306.21	J/mol×K	485.33	Joback Method
cpg	319.47	J/mol×K	516.24	Joback Method
cpg	332.17	J/mol×K	547.14	Joback Method
cpg	344.30	J/mol×K	578.05	Joback Method

cpg	355.88	J/mol×K	608.96	Joback Method
cpg	366.93	J/mol×K	639.87	Joback Method
cpg	377.46	J/mol×K	670.77	Joback Method
dvisc	0.0044834	Pa×s	243.27	Joback Method
dvisc	0.0018217	Pa×s	283.61	Joback Method
dvisc	0.0009263	Pa×s	323.96	Joback Method
dvisc	0.0005471	Pa×s	364.30	Joback Method
dvisc	0.0003589	Pa×s	404.64	Joback Method
dvisc	0.0002542	Pa×s	444.99	Joback Method
dvisc	0.0001906	Pa×s	485.33	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=R75624&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