

4-Hepten-2-ol, (E)-, 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-AATRIKPKSA-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	1013.00		NIST Webbook
rinpol	1014.00		NIST Webbook
rinpol	1013.00		NIST Webbook
tb	485.33	K	Joback Method
tc	670.77	K	Joback Method
tf	243.27	K	Joback Method
vc	0.537	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	306.21	J/mol×K	485.33	Joback Method
cpg	366.93	J/mol×K	639.87	Joback Method
cpg	355.88	J/mol×K	608.96	Joback Method
cpg	344.30	J/mol×K	578.05	Joback Method
cpg	332.17	J/mol×K	547.14	Joback Method
cpg	319.47	J/mol×K	516.24	Joback Method
cpg	377.46	J/mol×K	670.77	Joback Method

dvisc	0.0001906	Paxs	485.33	Joback Method
dvisc	0.0002542	Paxs	444.99	Joback Method
dvisc	0.0003589	Paxs	404.64	Joback Method
dvisc	0.0005471	Paxs	364.30	Joback Method
dvisc	0.0009263	Paxs	323.96	Joback Method
dvisc	0.0018217	Paxs	283.61	Joback Method
dvisc	0.0044834	Paxs	243.27	Joback Method

Sources

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=R75599&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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
mvol:	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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