hept-1-en-1-ol acetate

Other names: 1-heptenyl acetate
hept-1-en-1-ol acetate
hept-1-enyl acetate
Inchi: InChI=1S/C9H16O2/c1-3-4-5-6-7-8-11-9(2)10/h7-8H,3-6H2,1-2H3/b8-7+
InchiKey: JMFFUDMJDZXYCT-BQYQJAHWSA-N
Formula: C9H16O2
SMILES: CCCCC/C=C/OC(C)=O
Mol. weight [g/mol]: 156.23

Physical Properties

Property code	Value	Unit	Source
af	0.5241		Cheméo Relay (1.0)
gf	-128.80	kJ/mol	Joback Method
hf	-440.15	kJ/mol	Cheméo Relay (1.0)
hfus	22.06	kJ/mol	Joback Method
hvap	57.03	kJ/mol	Cheméo Relay (1.0)
ie	8.95	eV	Cheméo Relay (1.0)
log10ws	-3.26		Cheméo Relay (1.0)
logp	2.643		Crippen Method
mcvol	140.810	ml/mol	McGowan Method
pc	2540.49	kPa	Joback Method
rinpol	1234.00		NIST Webbook
rinpol	1234.00		NIST Webbook
ripol	1441.00		NIST Webbook
ripol	1444.00		NIST Webbook
ripol	1441.00		NIST Webbook
tb	456.64	K	Cheméo Relay (1.0)
tc	633.52	K	Cheméo Relay (1.0)
tf	218.18	K	Cheméo Relay (1.0)
vc	0.520	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source

cpg	306.02	J/mol×K	485.77	Joback Method
cpg	318.93	J/mol×K	516.03	Joback Method
cpg	331.30	J/mol×K	546.29	Joback Method
cpg	343.15	J/mol×K	576.54	Joback Method
cpg	354.47	J/mol×K	606.80	Joback Method
cpg	365.29	J/mol×K	637.06	Joback Method
cpg	375.62	J/mol×K	667.32	Joback Method
dvisc	0.0030655	Pa×s	258.27	Joback Method
dvisc	0.0014558	Pa×s	296.19	Joback Method
dvisc	0.0008186	Pa×s	334.10	Joback Method
dvisc	0.0005177	Pa×s	372.02	Joback Method
dvisc	0.0003563	Pa×s	409.94	Joback Method
dvisc	0.0002612	Pa×s	447.85	Joback Method
dvisc	0.0002011	Pa×s	485.77	Joback Method

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C35468974&Units=SI

Joback Method: https://en.wikipedia.org/wiki/Joback_method

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

Legend

af: Acentric Factor

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

ie: Ionization energy

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