3-Acetoxy-1-nonene

Other names: 1-Nonen-3-ol, acetate
1-nonen-3-yl acetate
1-hexylallyl acetate
Inchi: InChI=1S/C11H20O2/c1-4-6-7-8-9-11(5-2)13-10(3)12/h5,11H,2,4,6-9H2,1,3H3
InchiKey: PUWRLDPHAKKTKR-UHFFFAOYSA-N
Formula: C11H20O2
SMILES: C=CC(CCCCCC)OC(C)=O
Mol. weight [g/mol]: 184.28
CAS: 31795-37-6

Physical Properties

Property code	Value	Unit	Source
gf	-106.78	kJ/mol	Joback Method
hf	-395.02	kJ/mol	Joback Method
hfus	22.23	kJ/mol	Joback Method
hvap	48.18	kJ/mol	Joback Method
log10ws	-3.26		Crippen Method
logp	3.075		Crippen Method
mcvol	168.990	ml/mol	McGowan Method
pc	2108.07	kPa	Joback Method
rinpol	1175.00		NIST Webbook
rinpol	1175.00		NIST Webbook
ripol	1475.00		NIST Webbook
ripol	1477.00		NIST Webbook
ripol	1475.00		NIST Webbook
tb	523.61	K	Joback Method
tc	701.05	K	Joback Method
tf	269.13	K	Joback Method
vc	0.650	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	396.43	J/mol×K	523.61	Joback Method

cpg	411.21	J/mol×K	553.18	Joback Method
cpg	425.37	J/mol×K	582.76	Joback Method
cpg	438.94	J/mol×K	612.33	Joback Method
cpg	451.91	J/mol×K	641.90	Joback Method
cpg	464.30	J/mol×K	671.47	Joback Method
cpg	476.13	J/mol×K	701.05	Joback Method
dvisc	0.0041707	Pa×s	269.13	Joback Method
dvisc	0.0017765	Pa×s	311.54	Joback Method
dvisc	0.0009284	Pa×s	353.96	Joback Method
dvisc	0.0005575	Pa×s	396.37	Joback Method
dvisc	0.0003694	Pa×s	438.78	Joback Method
dvisc	0.0002632	Pa×s	481.20	Joback Method
dvisc	0.0001982	Pa×s	523.61	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=C31795376&Units=SI

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
ripol: Polar retention indices
tb: Normal Boiling Point Temperature
tc: Critical Temperature

tf: Normal melting (fusion) point

vc: Critical Volume