9-Decen-1-yl acetate

Other names:	Acetic acid 9-decenyl ester
	9-Decen-1-ol, acetate
	Decenyl acetate
	9-Decenyl acetate
Inchi:	InChI=1S/C12H22O2/c1-3-4-5-6-7-8-9-10-11-14-12(2)13/h3H,1,4-11H2,2H3
InchiKey:	PIQXMYAEJSMANF-UHFFFAOYSA-N
Formula:	C12H22O2
SMILES:	C=CCCCCCCCCOC(C)=O
Mol. weight [g/mol]:	198.30
CAS:	50816-18-7

Physical Properties

Property code	Value	Unit	Source
gf	-95.92	kJ/mol	Joback Method
hf	-410.38	kJ/mol	Joback Method
hfus	28.34	kJ/mol	Joback Method
hvap	50.79	kJ/mol	Joback Method
log10ws	-3.56		Crippen Method
logp	3.466		Crippen Method
mcvol	183.080	ml/mol	McGowan Method
pc	1920.30	kPa	Joback Method
rinpol	1359.00		NIST Webbook
rinpol	1399.30		NIST Webbook
rinpol	1431.00		NIST Webbook
rinpol	1378.60		NIST Webbook
rinpol	1383.00		NIST Webbook
ripol	1755.00		NIST Webbook
ripol	1755.00		NIST Webbook
ripol	1722.00		NIST Webbook
tb	546.93	K	Joback Method
tc	719.58	K	Joback Method
tf	295.40	K	Joback Method
vc	0.713	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	444.34	J/mol×K	546.93	Joback Method
cpg	459.51	J/mol×K	575.71	Joback Method
cpg	474.05	J/mol×K	604.48	Joback Method
cpg	487.98	J/mol×K	633.26	Joback Method
cpg	501.31	J/mol×K	662.03	Joback Method
cpg	514.06	J/mol×K	690.81	Joback Method
cpg	526.24	J/mol×K	719.58	Joback Method
dvisc	0.0029144	Pa×s	295.40	Joback Method
dvisc	0.0013996	Pa×s	337.32	Joback Method
dvisc	0.0007904	Pa×s	379.24	Joback Method
dvisc	0.0005002	Pa×s	421.17	Joback Method
dvisc	0.0003439	Pa×s	463.09	Joback Method
dvisc	0.0002516	Pa×s	505.01	Joback Method
dvisc	0.0001931	Pa×s	546.93	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=C50816187&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