7,9-dodecadien-1-ol, acetate

Inchi: InChI=1S/C14H24O2/c1-3-4-5-6-7-8-9-10-11-12-13-16-14(2)15/h4-7H,3,8-13H2,1-2H3/b
InchiKey: LLRZUAWETKPZJO-YTXTXJHMSA-N
Formula: C14H24O2
SMILES: CCC=CC=CCCCCCCOC(C)=O
Mol. weight [g/mol]: 224.34

Physical Properties

Property code	Value	Unit	Source
gf	-6.48	kJ/mol	Joback Method
hf	-342.65	kJ/mol	Joback Method
hfus	35.21	kJ/mol	Joback Method
hvap	55.83	kJ/mol	Joback Method
log10ws	-4.25		Crippen Method
logp	4.022		Crippen Method
mcvol	206.960	ml/mol	McGowan Method
pc	1718.88	kPa	Joback Method
rinpol	1602.00		NIST Webbook
tb	604.33	K	Joback Method
tc	784.52	K	Joback Method
tf	309.54	K	Joback Method
vc	0.803	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	527.63	J/mol×K	604.33	Joback Method
cpg	600.86	J/mol×K	754.48	Joback Method
cpg	587.61	J/mol×K	724.45	Joback Method
cpg	573.70	J/mol×K	694.42	Joback Method
cpg	559.08	J/mol×K	664.39	Joback Method
cpg	543.73	J/mol×K	634.36	Joback Method
cpg	613.47	J/mol×K	784.52	Joback Method
dvisc	0.0001119	Pa×s	604.33	Joback Method
dvisc	0.0001489	Pa×s	555.20	Joback Method

dvisc	0.0002093	Pa×s	506.07	Joback Method
dvisc	0.0003167	Pa×s	456.94	Joback Method
dvisc	0.0005296	Pa×s	407.80	Joback Method
dvisc	0.0010193	Pa×s	358.67	Joback Method
dvisc	0.0024152	Pa×s	309.54	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R308568&Units=SI
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

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

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