2,7-Octadien-1-ol, acetate, (E)-

Other names: (2E)-2,7-Octadienyl acetate
(E)-2,7-Octadien-1-yl acetate
Inchi: InChI=1S/C10H16O2/c1-3-4-5-6-7-8-9-12-10(2)11/h3,7-8H,1,4-6,9H2,2H3/b8-7+
InchiKey: RDOHPVPONNHSPH-BQYQJAHWSA-N
Formula: C10H16O2
SMILES: C=CCCCC=CCOC(C)=O
Mol. weight [g/mol]: 168.23
CAS: 30460-73-2

Physical Properties

Property code	Value	Unit	Source
gf	-32.54	kJ/mol	Joback Method
hf	-251.88	kJ/mol	Joback Method
hfus	23.37	kJ/mol	Joback Method
hvap	46.30	kJ/mol	Joback Method
log10ws	-2.58		Crippen Method
logp	2.462		Crippen Method
mcvol	150.600	ml/mol	McGowan Method
pc	2407.64	kPa	Joback Method
rinpol	1388.00		NIST Webbook
tb	505.33	K	Joback Method
tc	688.59	K	Joback Method
tf	267.78	K	Joback Method
vc	0.581	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	332.46	J/mol×K	505.33	Joback Method
cpg	345.70	J/mol×K	535.87	Joback Method
cpg	358.33	J/mol×K	566.42	Joback Method
cpg	370.39	J/mol×K	596.96	Joback Method
cpg	381.88	J/mol×K	627.50	Joback Method
cpg	392.82	J/mol×K	658.05	Joback Method

cpg	403.24	J/mol×K	688.59	Joback Method
dvisc	0.0028123	Pa×s	267.78	Joback Method
dvisc	0.0013463	Pa×s	307.37	Joback Method
dvisc	0.0007625	Pa×s	346.96	Joback Method
dvisc	0.0004852	Pa×s	386.55	Joback Method
dvisc	0.0003358	Pa×s	426.15	Joback Method
dvisc	0.0002474	Pa×s	465.74	Joback Method
dvisc	0.0001912	Pa×s	505.33	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=C30460732&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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