Phenol, 4-[3-(acetyloxy)-1-propenyl]-2-methoxy-, acetate

Other names: Coniferyl alcohol, diacetate
Inchi: InChI=1S/C14H16O5/c1-10(15)18-8-4-5-12-6-7-13(19-11(2)16)14(9-12)17-3/h4-7,9H,8H
InchiKey: KCODNVFFXXYJPA-PLNGDYQASA-N
Formula: C14H16O5
SMILES: COc1cc(C=CCOC(C)=O)ccc1OC(C)=O
Mol. weight [g/mol]: 264.27
CAS: 38209-46-0

Physical Properties

Property code	Value	Unit	Source
gf	-332.47	kJ/mol	Joback Method
hf	-623.30	kJ/mol	Joback Method
hfus	32.24	kJ/mol	Joback Method
hvap	71.04	kJ/mol	Joback Method
log10ws	-2.85		Crippen Method
logp	2.197		Crippen Method
mcvol	200.810	ml/mol	McGowan Method
pc	2195.89	kPa	Joback Method
rinpol	2030.40		NIST Webbook
rinpol	2030.40		NIST Webbook
tb	735.52	K	Joback Method
tc	947.64	K	Joback Method
tf	460.47	K	Joback Method
vc	0.757	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	541.46	J/mol×K	735.52	Joback Method
cpg	599.48	J/mol×K	912.28	Joback Method
cpg	589.67	J/mol×K	876.93	Joback Method
cpg	578.96	J/mol×K	841.58	Joback Method
cpg	567.35	J/mol×K	806.23	Joback Method
cpg	554.85	J/mol×K	770.87	Joback Method

cpg	608.40	J/mol×K	947.64	Joback Method
dvisc	0.0000797	Pa×s	735.52	Joback Method
dvisc	0.0000989	Pa×s	689.68	Joback Method
dvisc	0.0001267	Pa×s	643.84	Joback Method
dvisc	0.0001685	Pa×s	598.00	Joback Method
dvisc	0.0002349	Pa×s	552.15	Joback Method
dvisc	0.0003478	Pa×s	506.31	Joback Method
dvisc	0.0005570	Pa×s	460.47	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=C38209460&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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