(E)-3-(4-Acetoxyphenyl)allyl acetate

Inchi: InChI=1S/C13H14O4/c1-10(14)16-9-3-4-12-5-7-13(8-6-12)17-11(2)15/h3-8H,9H2,1-2H3/
InchiKey: JAFORXKRQBIDEE-ONEGZZNKSA-N
Formula: C13H14O4
SMILES: CC(=O)OCC=Cc1ccc(OC(C)=O)cc1
Mol. weight [g/mol]: 234.25
CAS: 113944-48-2

Physical Properties

Property code	Value	Unit	Source
gf	-226.26	kJ/mol	Joback Method
hf	-458.97	kJ/mol	Joback Method
hfus	28.85	kJ/mol	Joback Method
hvap	65.74	kJ/mol	Joback Method
log10ws	-2.73		Crippen Method
logp	2.188		Crippen Method
mcvol	180.850	ml/mol	McGowan Method
pc	2485.07	kPa	Joback Method
rinpol	1847.20		NIST Webbook
rinpol	1847.20		NIST Webbook
tb	685.24	K	Joback Method
tc	901.78	K	Joback Method
tf	414.45	K	Joback Method
vc	0.683	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	464.71	J/mol×K	685.24	Joback Method
cpg	478.02	J/mol×K	721.33	Joback Method
cpg	490.47	J/mol×K	757.42	Joback Method
cpg	502.06	J/mol×K	793.51	Joback Method
cpg	512.82	J/mol×K	829.60	Joback Method
cpg	522.76	J/mol×K	865.69	Joback Method
cpg	531.91	J/mol×K	901.78	Joback Method

dvisc	0.0009651	Pa×s	414.45	Joback Method
dvisc	0.0005691	Pa×s	459.58	Joback Method
dvisc	0.0003688	Pa×s	504.71	Joback Method
dvisc	0.0002566	Pa×s	549.85	Joback Method
dvisc	0.0001887	Pa×s	594.98	Joback Method
dvisc	0.0001449	Pa×s	640.11	Joback Method
dvisc	0.0001152	Pa×s	685.24	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=C113944482&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