(S)-4-(1-Acetoxyallyl)phenyl acetate

Inchi: InChI=1S/C13H14O4/c1-4-13(17-10(3)15)11-5-7-12(8-6-11)16-9(2)14/h4-8,13H,1H2,2-3
InchiKey: JAMQIUWGGBSIKZ-CYBMUJFWSA-N
Formula: C13H14O4
SMILES: C=CC(OC(C)=O)c1ccc(OC(C)=O)cc1
Mol. weight [g/mol]: 234.25
CAS: 52946-22-2

Physical Properties

Property code	Value	Unit	Source
gf	-221.08	kJ/mol	Joback Method
hf	-456.04	kJ/mol	Joback Method
hfus	23.85	kJ/mol	Joback Method
hvap	64.72	kJ/mol	Joback Method
log10ws	-3.02		Crippen Method
logp	2.402		Crippen Method
mcvol	180.850	ml/mol	McGowan Method
pc	2480.12	kPa	Joback Method
rinpol	1649.50		NIST Webbook
rinpol	1649.50		NIST Webbook
tb	677.32	K	Joback Method
tc	893.68	K	Joback Method
tf	402.77	K	Joback Method
vc	0.678	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	465.07	J/mol×K	677.32	Joback Method
cpg	478.64	J/mol×K	713.38	Joback Method
cpg	491.31	J/mol×K	749.44	Joback Method
cpg	503.10	J/mol×K	785.50	Joback Method
cpg	514.02	J/mol×K	821.56	Joback Method
cpg	524.07	J/mol×K	857.62	Joback Method
cpg	533.27	J/mol×K	893.68	Joback Method

dvisc	0.0012222	Pa×s	402.77	Joback Method
dvisc	0.0006955	Pa×s	448.53	Joback Method
dvisc	0.0004393	Pa×s	494.29	Joback Method
dvisc	0.0002999	Pa×s	540.04	Joback Method
dvisc	0.0002174	Pa×s	585.80	Joback Method
dvisc	0.0001651	Pa×s	631.56	Joback Method
dvisc	0.0001301	Pa×s	677.32	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=C52946222&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