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

Inchi: InChI=1S/C11H12O3/c1-3-11(13)9-4-6-10(7-5-9)14-8(2)12/h3-7,11,13H,1H2,2H3/t11-/m1
InchiKey: GKYVDAMMLMMJGZ-LLVKDONJSA-N
Formula: C11H12O3
SMILES: C=CC(O)c1ccc(OC(C)=O)cc1
Mol. weight [g/mol]: 192.21
CAS: 343583-65-3

Physical Properties

Property code	Value	Unit	Source
gf	-140.82	kJ/mol	Joback Method
hf	-322.19	kJ/mol	Joback Method
hfus	19.97	kJ/mol	Joback Method
hvap	67.80	kJ/mol	Joback Method
log10ws	-2.58		Crippen Method
logp	1.831		Crippen Method
mcvol	151.100	ml/mol	McGowan Method
pc	3191.93	kPa	Joback Method
rinpol	1550.20		NIST Webbook
rinpol	1550.20		NIST Webbook
tb	647.45	K	Joback Method
tc	851.46	K	Joback Method
tf	368.89	K	Joback Method
vc	0.561	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	377.46	J/mol×K	647.45	Joback Method
cpg	388.70	J/mol×K	681.45	Joback Method
cpg	399.26	J/mol×K	715.45	Joback Method
cpg	409.15	J/mol×K	749.45	Joback Method
cpg	418.40	J/mol×K	783.46	Joback Method
cpg	427.03	J/mol×K	817.46	Joback Method
cpg	435.05	J/mol×K	851.46	Joback Method

dvisc	0.0028895	Pa×s	368.89	Joback Method
dvisc	0.0010347	Pa×s	415.32	Joback Method
dvisc	0.0004555	Pa×s	461.74	Joback Method
dvisc	0.0002330	Pa×s	508.17	Joback Method
dvisc	0.0001333	Pa×s	554.60	Joback Method
dvisc	0.0000832	Pa×s	601.02	Joback Method
dvisc	0.0000555	Pa×s	647.45	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C343583653&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

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