(E)-4-(3-Hydroxyprop-1-en-1-yl)phenyl acetate

Inchi: InChI=1S/C11H12O3/c1-9(13)14-11-6-4-10(5-7-11)3-2-8-12/h2-7,12H,8H2,1H3/b3-2+
InchiKey: MUHNYWKQFOFBRC-NSCUHMNNSA-N
Formula: C11H12O3
SMILES: CC(=O)Oc1ccc(C=CCO)cc1
Mol. weight [g/mol]: 192.21
CAS: 94723-93-0

Physical Properties

Property code	Value	Unit	Source
gf	-146.00	kJ/mol	Joback Method
hf	-325.12	kJ/mol	Joback Method
hfus	24.98	kJ/mol	Joback Method
hvap	68.81	kJ/mol	Joback Method
log10ws	-2.29		Crippen Method
logp	1.617		Crippen Method
mcvol	151.100	ml/mol	McGowan Method
pc	3199.16	kPa	Joback Method
rinpol	1714.00		NIST Webbook
rinpol	1714.00		NIST Webbook
tb	655.37	K	Joback Method
tc	859.69	K	Joback Method
tf	380.57	K	Joback Method
vc	0.567	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	376.78	J/mol×K	655.37	Joback Method
cpg	387.81	J/mol×K	689.42	Joback Method
cpg	398.16	J/mol×K	723.48	Joback Method
cpg	407.88	J/mol×K	757.53	Joback Method
cpg	416.98	J/mol×K	791.59	Joback Method
cpg	425.49	J/mol×K	825.64	Joback Method
cpg	433.44	J/mol×K	859.69	Joback Method

dvisc	0.0020128	Pa×s	380.57	Joback Method
dvisc	0.0007726	Pa×s	426.37	Joback Method
dvisc	0.0003571	Pa×s	472.17	Joback Method
dvisc	0.0001892	Pa×s	517.97	Joback Method
dvisc	0.0001111	Pa×s	563.77	Joback Method
dvisc	0.0000707	Pa×s	609.57	Joback Method
dvisc	0.0000479	Pa×s	655.37	Joback Method

Sources

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=C94723930&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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