1-(4-Acetoxy-3-methoxyphenyl)allyl acetate

Inchi: InChI=1S/C14H16O5/c1-5-12(18-9(2)15)11-6-7-13(19-10(3)16)14(8-11)17-4/h5-8,12H,1H
InchiKey: NKRBAUXTIWONOV-UHFFFAOYSA-N
Formula: C14H16O5
SMILES: C=CC(OC(C)=O)c1ccc(OC(C)=O)c(OC)c1
Mol. weight [g/mol]: 264.27
CAS: 53890-24-7

Physical Properties

Property code	Value	Unit	Source
gf	-327.29	kJ/mol	Joback Method
hf	-620.37	kJ/mol	Joback Method
hfus	27.24	kJ/mol	Joback Method
hvap	70.02	kJ/mol	Joback Method
log10ws	-3.14		Crippen Method
logp	2.411		Crippen Method
mcvol	200.810	ml/mol	McGowan Method
pc	2191.78	kPa	Joback Method
rinpol	1799.90		NIST Webbook
rinpol	1799.90		NIST Webbook
tb	727.60	K	Joback Method
tc	939.45	K	Joback Method
tf	448.79	K	Joback Method
vc	0.752	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	541.83	J/mol×K	727.60	Joback Method
cpg	555.45	J/mol×K	762.91	Joback Method
cpg	568.14	J/mol×K	798.22	Joback Method
cpg	579.91	J/mol×K	833.53	Joback Method
cpg	590.73	J/mol×K	868.83	Joback Method
cpg	600.61	J/mol×K	904.14	Joback Method
cpg	609.52	J/mol×K	939.45	Joback Method

dvisc	0.0006915	Pa×s	448.79	Joback Method
dvisc	0.0004195	Pa×s	495.26	Joback Method
dvisc	0.0002773	Pa×s	541.73	Joback Method
dvisc	0.0001956	Pa×s	588.20	Joback Method
dvisc	0.0001453	Pa×s	634.66	Joback Method
dvisc	0.0001124	Pa×s	681.13	Joback Method
dvisc	0.0000898	Pa×s	727.60	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=C53890247&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