(E)-4-(3,4-Dimethoxyphenyl)but-3-en-1-yl acetate

Inchi: InChI=1S/C14H18O4/c1-11(15)18-9-5-4-6-12-7-8-13(16-2)14(10-12)17-3/h4,6-8,10H,5,9

InchiKey: LTWAPTPDRUNVGD-GQCTYLIASA-N

Formula: C14H18O4

SMILES: COc1ccc(C=CCCOC(C)=O)cc1OC

Mol. weight [g/mol]: 250.29

CAS: 69768-98-5

Physical Properties

Property code	Value	Unit	Source
gf	-203.55	kJ/mol	Joback Method
hf	-510.72	kJ/mol	Joback Method
hfus	30.64	kJ/mol	Joback Method
hvap	64.29	kJ/mol	Joback Method
log10ws	-3.07		Crippen Method
logp	2.670		Crippen Method
mcvol	199.240	ml/mol	McGowan Method
pc	2071.76	kPa	Joback Method
rinpol	1993.70		NIST Webbook
rinpol	1993.70		NIST Webbook
tb	681.65	K	Joback Method
tc	887.45	K	Joback Method
tf	410.54	K	Joback Method
vc	0.751	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	525.23	J/mol×K	681.65	Joback Method
cpg	540.08	J/mol×K	715.95	Joback Method
cpg	554.09	J/mol×K	750.25	Joback Method
cpg	567.26	J/mol×K	784.55	Joback Method
cpg	579.59	J/mol×K	818.85	Joback Method
cpg	591.10	J/mol×K	853.15	Joback Method
cpg	601.76	J/mol×K	887.45	Joback Method

dvisc	0.0006339	Pa×s	410.54	Joback Method
dvisc	0.0003773	Pa×s	455.73	Joback Method
dvisc	0.0002466	Pa×s	500.91	Joback Method
dvisc	0.0001730	Pa×s	546.10	Joback Method
dvisc	0.0001280	Pa×s	591.28	Joback Method
dvisc	0.0000989	Pa×s	636.47	Joback Method
dvisc	0.0000791	Pa×s	681.65	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C69768985&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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