4-(2-formylvinyl)-2-methoxyphenyl acetate

Other names: (E)-2-Methoxy-4-(3-oxoprop-1-en-1-yl)phenyl acetate
Inchi: InChI=1S/C12H12O4/c1-9(14)16-11-6-5-10(4-3-7-13)8-12(11)15-2/h3-8H,1-2H3/b4-3+
InchiKey: VEKAJHBFBMWJKI-ONEGZZNKSA-N
Formula: C12H12O4
SMILES: COc1cc(C=CC=O)ccc1OC(C)=O
Mol. weight [g/mol]: 220.22
CAS: 65401-83-4

Physical Properties

Property code	Value	Unit	Source
gf	-214.91	kJ/mol	Joback Method
hf	-422.80	kJ/mol	Joback Method
hfus	26.57	kJ/mol	Joback Method
hvap	64.15	kJ/mol	Joback Method
log10ws	-2.43		Crippen Method
logp	1.833		Crippen Method
mcvol	166.760	ml/mol	McGowan Method
pc	2729.71	kPa	Joback Method
rinpol	1861.30		NIST Webbook
tb	662.13	K	Joback Method
tc	878.68	K	Joback Method
tf	407.77	K	Joback Method
vc	0.638	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	413.77	J/mol×K	662.13	Joback Method
cpg	426.05	J/mol×K	698.22	Joback Method
cpg	437.58	J/mol×K	734.31	Joback Method
cpg	448.36	J/mol×K	770.40	Joback Method
cpg	458.40	J/mol×K	806.49	Joback Method
cpg	467.71	J/mol×K	842.59	Joback Method
cpg	476.30	J/mol×K	878.68	Joback Method

dvisc	0.0009540	Pa×s	407.77	Joback Method
dvisc	0.0005969	Pa×s	450.16	Joback Method
dvisc	0.0004049	Pa×s	492.56	Joback Method
dvisc	0.0002920	Pa×s	534.95	Joback Method
dvisc	0.0002210	Pa×s	577.34	Joback Method
dvisc	0.0001737	Pa×s	619.74	Joback Method
dvisc	0.0001409	Pa×s	662.13	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=C65401834&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