Phenol, 2-methoxy-4-(1-propenyl)-, acetate, (e)-

Other names:	2-Methoxy-4-[(1E)-1-propenyl]phenyl acetate
	Isoeugenol acetate (E)
	trans-Isoeugenol acetate
	Phenol, 2-methoxy-4-propenyl-, acetate, (E)-
	isoeugenyl acetate 1
Inchi:	InChI=1S/C12H14O3/c1-4-5-10-6-7-11(15-9(2)13)12(8-10)14-3/h4-8H,1-3H3/b5-4-
InchiKey:	IUSBVFZKQJGVEP-SNAWJCMRSA-N
Formula:	C12H14O3
SMILES:	C/C=C/c1ccc(OC(C)=O)c(OC)c1
Mol. weight [g/mol]:	206.24

Physical Properties

Property code	Value	Unit	Source
hfus	24.28	kJ/mol	Joback Method
hvap	77.95	kJ/mol	Cheméo Relay (1.0)
ie	7.56	eV	Cheméo Relay (1.0)
log10ws	-3.30		Cheméo Relay (1.0)
logp	2.654		Crippen Method
mcvol	165.190	ml/mol	McGowan Method
rinpol	1534.40		NIST Webbook
rinpol	1617.00		NIST Webbook
rinpol	1617.00		NIST Webbook
tb	564.16	K	Cheméo Relay (1.0)
tf	335.07	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	398.09	J/mol×K	613.47	Joback Method
cpg	411.97	J/mol×K	649.20	Joback Method
cpg	425.09	J/mol×K	684.94	Joback Method
cpg	437.45	J/mol×K	720.67	Joback Method
cpg	449.08	J/mol×K	756.41	Joback Method
cpg	459.96	J/mol×K	792.14	Joback Method

cpg	470.13	J/mol×K	827.88	Joback Method
dvisc	0.0009291	Pa×s	365.77	Joback Method
dvisc	0.0005581	Pa×s	407.05	Joback Method
dvisc	0.0003683	Pa×s	448.34	Joback Method
dvisc	0.0002607	Pa×s	489.62	Joback Method
dvisc	0.0001947	Pa×s	530.90	Joback Method
dvisc	0.0001516	Pa×s	572.19	Joback Method
dvisc	0.0001222	Pa×s	613.47	Joback Method

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):
Cheméo Relay (1.0, beta):
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C5912878&Units=SI
Joback Method: https://en.wikipedia.org/wiki/Joback_method
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

cpg: Ideal gas heat capacity
dvisc: Dynamic viscosity
hfus: Enthalpy of fusion at standard conditions
hvap: Enthalpy of vaporization at standard conditions
ie: Ionization energy
log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
rinpol: Non-polar retention indices
tb: Normal Boiling Point Temperature
tf: Normal melting (fusion) point