

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

Other names:	Phenol, 2-methoxy-4-propenyl-, acetate Acetisoeugenol Acetylisoeugenol Isoeugenol, acetate Isoeugenyl acetate 2-Methoxy-4-propenylphenyl acetate Acetisoeugenol 4-Acetoxy-3-methoxy-1-propenylbenzene 2-Methoxy-4-(1-propenyl)phenyl acetate NSC 46121 O-Acetylisoeugenol Phenol, 2-methoxy-4-(1-propen-1-yl)-, 1-acetate 2-methoxy-4-prop-1-enylphenyl acetate
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:	CC=Cc1ccc(OC(C)=O)c(OC)c1
Mol. weight [g/mol]:	206.24
CAS:	93-29-8

Physical Properties

Property code	Value	Unit	Source
gf	-115.39	kJ/mol	Joback Method
hf	-337.22	kJ/mol	Joback Method
hfus	24.28	kJ/mol	Joback Method
hvap	57.43	kJ/mol	Joback Method
log10ws	-3.15		Crippen Method
logp	2.654		Crippen Method
mcvol	165.190	ml/mol	McGowan Method
pc	2530.27	kPa	Joback Method
rinpol	1620.00		NIST Webbook
rinpol	1614.00		NIST Webbook
rinpol	1620.00		NIST Webbook
rinpol	1614.00		NIST Webbook
ripol	2395.00		NIST Webbook
ripol	2395.00		NIST Webbook
tb	613.47	K	Joback Method

tc	827.88	K	Joback Method
tf	365.77	K	Joback Method
vc	0.622	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	398.09	J/mol×K	613.47	Joback Method
cpg	459.96	J/mol×K	792.14	Joback Method
cpg	449.08	J/mol×K	756.41	Joback Method
cpg	437.45	J/mol×K	720.67	Joback Method
cpg	425.09	J/mol×K	684.94	Joback Method
cpg	411.97	J/mol×K	649.20	Joback Method
cpg	470.13	J/mol×K	827.88	Joback Method
dvisc	0.0001222	Paxs	613.47	Joback Method
dvisc	0.0001516	Paxs	572.19	Joback Method
dvisc	0.0001947	Paxs	530.90	Joback Method
dvisc	0.0002607	Paxs	489.62	Joback Method
dvisc	0.0003683	Paxs	448.34	Joback Method
dvisc	0.0005581	Paxs	407.05	Joback Method
dvisc	0.0009291	Paxs	365.77	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C93298&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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