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

Other names:	Phenol, 4-allyl-2-methoxy-, acetate
	Aceteugenol
	Acetyleugenol
	Eugenol acetate
	Eugenyl acetate
	1,3,4-Eugenol acetate
	Aceto eugenol
	1-Acetoxy-2-methoxy-4-allylbenzene
	4-Allyl-2-methoxyphenol acetate
	4-Allyl-2-methoxyphenyl acetate
	NSC 1242
	Phenol, 2-methoxy-4-(2-propen-1-yl)-, 1-acetate
Inchi:	InChI=1S/C12H14O3/c1-4-5-10-6-7-11(15-9(2)13)12(8-10)14-3/h4,6-8H,1,5H2,2-3H3
InchiKey:	SCCDQYPEOIRVGX-UHFFFAOYSA-N
Formula:	C12H14O3
SMILES:	C=CCc1ccc(OC(C)=O)c(OC)c1
Mol. weight [g/mol]:	206.24
CAS:	93-28-7

Physical Properties

Property code	Value	Unit	Source
gf	-107.77	kJ/mol	Joback Method
hf	-329.01	kJ/mol	Joback Method
hfus	22.79	kJ/mol	Joback Method
hvap	56.80	kJ/mol	Joback Method
log10ws	-2.98		Crippen Method
logp	2.349		Crippen Method
mcvol	165.190	ml/mol	McGowan Method
pc	2505.01	kPa	Joback Method
rinpol	1483.00		NIST Webbook
rinpol	1486.00		NIST Webbook
rinpol	1523.00		NIST Webbook
rinpol	1526.00		NIST Webbook
rinpol	1531.00		NIST Webbook
rinpol	1522.00		NIST Webbook
rinpol	1485.00		NIST Webbook
rinpol	1524.00		NIST Webbook

rinpol	1474.00		NIST Webbook
rinpol	1484.00		NIST Webbook
rinpol	1485.00		NIST Webbook
rinpol	1520.00		NIST Webbook
rinpol	1482.00		NIST Webbook
rinpol	1526.00		NIST Webbook
rinpol	1524.00		NIST Webbook
rinpol	1514.00		NIST Webbook
rinpol	1523.00		NIST Webbook
rinpol	1541.00		NIST Webbook
rinpol	1522.00		NIST Webbook
rinpol	1493.00		NIST Webbook
rinpol	1493.00		NIST Webbook
rinpol	1526.00		NIST Webbook
rinpol	1523.00		NIST Webbook
rinpol	1524.00		NIST Webbook
rinpol	1520.00		NIST Webbook
rinpol	1526.00		NIST Webbook
rinpol	1486.00		NIST Webbook
rinpol	1524.00		NIST Webbook
rinpol	1482.00		NIST Webbook
rinpol	1525.00		NIST Webbook
rinpol	1485.00		NIST Webbook
rinpol	1525.00		NIST Webbook
rinpol	1482.00		NIST Webbook
rinpol	1483.00		NIST Webbook
ripol	2263.00		NIST Webbook
ripol	2263.00		NIST Webbook
ripol	2263.00		NIST Webbook
ripol	2273.00		NIST Webbook
ripol	2252.00		NIST Webbook
ripol	2277.00		NIST Webbook
ripol	2273.00		NIST Webbook
tb	605.99	K	Joback Method
tc	815.85	K	Joback Method
tf	369.09	K	Joback Method
vc	0.623	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source

cpg	397.71	J/mol×K	605.99	Joback Method
cpg	411.50	J/mol×K	640.97	Joback Method
cpg	424.56	J/mol×K	675.94	Joback Method
cpg	436.90	J/mol×K	710.92	Joback Method
cpg	448.51	J/mol×K	745.90	Joback Method
cpg	459.40	J/mol×K	780.88	Joback Method
cpg	469.57	J/mol×K	815.85	Joback Method
dvisc	0.0009921	Pa×s	369.09	Joback Method
dvisc	0.0006199	Pa×s	408.57	Joback Method
dvisc	0.0004207	Pa×s	448.06	Joback Method
dvisc	0.0003041	Pa×s	487.54	Joback Method
dvisc	0.0002307	Pa×s	527.02	Joback Method
dvisc	0.0001819	Pa×s	566.51	Joback Method
dvisc	0.0001480	Pa×s	605.99	Joback Method
hvapt	63.10	kJ/mol	464.50	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	554.20	K	100.00	NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C93287&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
hvapt:	Enthalpy of vaporization at a given temperature
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
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume