Phenol, 2-methoxy-, acetate

Other names:	Phenol, o-methoxy-, acetate
	o-Acetoxyanisole
	o-Methoxyphenyl acetate
	Eucol
	Guaiacol acetate
	Guaiacyl acetate
	1-Acetoxy-2-methoxybenzene
	2-Methoxyphenyl acetate
	o-Anisyl acetate
	2-Acetoxyanisole
	NSC 3831
	O-Acetylguaiacol
	Phenol, 2-methoxy-, 1-acetate
	Guaiaol acetate
	Acetic acid, 2-methoxyphenyl ester
Inchi:	InChI=1S/C9H10O3/c1-7(10)12-9-6-4-3-5-8(9)11-2/h3-6H,1-2H3
InchiKey:	BHJHPYFAYGAPLS-UHFFFAOYSA-N
Formula:	C9H10O3
SMILES:	COc1ccccc1OC(C)=O
Mol. weight [g/mol]:	166.17
CAS:	613-70-7

Physical Properties

Property code	Value	Unit	Source
gf	-211.24	kJ/mol	Joback Method
hf	-381.05	kJ/mol	Joback Method
hfus	16.69	kJ/mol	Joback Method
hvap	50.13	kJ/mol	Joback Method
log10ws	-1.90		Crippen Method
logp	1.620		Crippen Method
mcvol	127.220	ml/mol	McGowan Method
pc	3314.37	kPa	Joback Method
rinpol	1195.00		NIST Webbook
ripol	2123.00		NIST Webbook
ripol	2123.00		NIST Webbook
tb	535.69	K	Joback Method
tc	750.72	K	Joback Method

tf	324.52	K	Joback Method
vc	0.473	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	278.97	J/mol×K	535.69	Joback Method
cpg	291.01	J/mol×K	571.53	Joback Method
cpg	302.48	J/mol×K	607.37	Joback Method
cpg	313.35	J/mol×K	643.20	Joback Method
cpg	323.62	J/mol×K	679.04	Joback Method
cpg	333.30	J/mol×K	714.88	Joback Method
cpg	342.37	J/mol×K	750.72	Joback Method
dvisc	0.0013483	Pa×s	324.52	Joback Method
dvisc	0.0008247	Pa×s	359.72	Joback Method
dvisc	0.0005507	Pa×s	394.91	Joback Method
dvisc	0.0003928	Pa×s	430.11	Joback Method
dvisc	0.0002949	Pa×s	465.30	Joback Method
dvisc	0.0002305	Pa×s	500.50	Joback Method
dvisc	0.0001861	Pa×s	535.69	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	396.20	K	2.40	NIST Webbook
tbrp	396.70	K	1.70	NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C613707&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
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