Phenol, 3-methoxy-, acetate

Other names:	Phenol, m-methoxy-, acetate
	m-Acetoxyanisole
	m-Methoxyphenyl acetate
	3-Methoxyphenyl acetate
	3-Methoxyphenol, acetate
Inchi:	InChI=1S/C9H10O3/c1-7(10)12-9-5-3-4-8(6-9)11-2/h3-6H,1-2H3
InchiKey:	QQYNGKGFOZQMHD-UHFFFAOYSA-N
Formula:	C9H10O3
SMILES:	COc1cccc(OC(C)=O)c1
Mol. weight [g/mol]:	166.17
CAS:	5451-83-2

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
ie	8.30 ± 0.20	eV	NIST Webbook
log10ws	-1.90		Crippen Method
logp	1.620		Crippen Method
mcvol	127.220	ml/mol	McGowan Method
pc	3314.37	kPa	Joback Method
rinpol	1313.40		NIST Webbook
rinpol	1313.40		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	333.30	J/mol×K	714.88	Joback Method
cpg	323.62	J/mol×K	679.04	Joback Method
cpg	313.35	J/mol×K	643.20	Joback Method
cpg	302.48	J/mol×K	607.37	Joback Method
cpg	291.01	J/mol×K	571.53	Joback Method
cpg	342.37	J/mol×K	750.72	Joback Method
dvisc	0.0001861	Pa×s	535.69	Joback Method
dvisc	0.0002305	Pa×s	500.50	Joback Method
dvisc	0.0002949	Pa×s	465.30	Joback Method
dvisc	0.0003928	Pa×s	430.11	Joback Method
dvisc	0.0005507	Pa×s	394.91	Joback Method
dvisc	0.0008247	Pa×s	359.72	Joback Method
dvisc	0.0013483	Pa×s	324.52	Joback Method

Sources

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
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C5451832&Units=SI

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
ie: Ionization energy
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