

Phenol, 4-methoxy-, acetate

Other names:	Phenol, p-methoxy-, acetate p-Acetoxyanisole p-Methoxyphenyl acetate 4-Methoxyphenyl acetate 4-Methoxyphenol, acetate
Inchi:	InChI=1S/C9H10O3/c1-7(10)12-9-5-3-8(11-2)4-6-9/h3-6H,1-2H3
InchiKey:	YAPCNXGBNRDBIW-UHFFFAOYSA-N
Formula:	C9H10O3
SMILES:	COc1ccc(OC(C)=O)cc1
Mol. weight [g/mol]:	166.17
CAS:	1200-06-2

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	7.90 ± 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	1324.00		NIST Webbook
rinpol	1324.00		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

Sources

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=C1200062&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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

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