Vanillin, acetate

Other names:	Benzaldehyde, 4-(acetyloxy)-3-methoxy-
	Acetovanillin
	Acetylvanillin
	O-Acetylvanillin
	4-Acetoxy-3-methoxybenzaldehyde
	4-O-Acetylvanillin
	4-Formyl-2-methoxyphenol acetate
	4-Formyl-2-methoxyphenyl acetate
	Benzaldehyde, 4-acetoxy-3-methoxy
	4-(Acetyloxy)-3-methoxybenzaldehyde
	NSC 25863
	NSC 8499
Inchi:	InChI=1S/C10H10O4/c1-7(12)14-9-4-3-8(6-11)5-10(9)13-2/h3-6H,1-2H3
InchiKey:	PZSJOBKRSVRODF-UHFFFAOYSA-N
Formula:	C10H10O4
SMILES:	COc1cc(C=O)ccc1OC(C)=O
Mol. weight [g/mol]:	194.18
CAS:	881-68-5

Physical Properties

Property code	Value	Unit	Source
gf	-311.97	kJ/mol	Joback Method
hf	-498.74	kJ/mol	Joback Method
hfus	21.18	kJ/mol	Joback Method
hvap	59.74	kJ/mol	Joback Method
log10ws	-2.15		Crippen Method
logp	1.433		Crippen Method
mcvol	142.880	ml/mol	McGowan Method
pc	3177.55	kPa	Joback Method
rinpol	1512.00		NIST Webbook
rinpol	258.80		NIST Webbook
rinpol	1540.80		NIST Webbook
rinpol	1465.00		NIST Webbook
rinpol	1512.00		NIST Webbook
tb	612.21	K	Joback Method
tc	827.41	K	Joback Method
tf	390.31	K	Joback Method

vc	0.546	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	338.79	J/mol×K	612.21	Joback Method
cpg	389.47	J/mol×K	791.54	Joback Method
cpg	380.62	J/mol×K	755.68	Joback Method
cpg	371.12	J/mol×K	719.81	Joback Method
cpg	360.97	J/mol×K	683.94	Joback Method
cpg	350.19	J/mol×K	648.08	Joback Method
cpg	397.65	J/mol×K	827.41	Joback Method
dvisc	0.0001978	Pa×s	612.21	Joback Method
dvisc	0.0002406	Pa×s	575.23	Joback Method
dvisc	0.0003007	Pa×s	538.24	Joback Method
dvisc	0.0003883	Pa×s	501.26	Joback Method
dvisc	0.0005224	Pa×s	464.28	Joback Method
dvisc	0.0007397	Pa×s	427.29	Joback Method
dvisc	0.0011188	Pa×s	390.31	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=C881685&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
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