

4-Hydroxy-2-methoxybenzaldehyde, acetate

Inchi:	InChI=1S/C10H10O4/c1-7(12)14-9-4-3-8(6-11)10(5-9)13-2/h3-6H,1-2H3
InchiKey:	PPIOKNUCIBXREP-UHFFFAOYSA-N
Formula:	C10H10O4
SMILES:	<chem>COc1cc(OC(C)=O)ccc1C=O</chem>
Mol. weight [g/mol]:	194.18

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
mvol	142.880	ml/mol	McGowan Method
pc	3177.55	kPa	Joback Method
rinpol	1618.60		NIST Webbook
rinpol	1618.60		NIST Webbook
tb	612.21	K	Joback Method
tc	827.41	K	Joback Method
tf	390.31	K	Joback Method
vc	0.546	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	338.79	J/molxK	612.21	Joback Method
cpg	350.19	J/molxK	648.08	Joback Method
cpg	360.97	J/molxK	683.94	Joback Method
cpg	371.12	J/molxK	719.81	Joback Method
cpg	380.62	J/molxK	755.68	Joback Method
cpg	389.47	J/molxK	791.54	Joback Method
cpg	397.65	J/molxK	827.41	Joback Method
dvisc	0.0011188	Paxs	390.31	Joback Method

dvisc	0.0007397	Paxs	427.29	Joback Method
dvisc	0.0005224	Paxs	464.28	Joback Method
dvisc	0.0003883	Paxs	501.26	Joback Method
dvisc	0.0003007	Paxs	538.24	Joback Method
dvisc	0.0002406	Paxs	575.23	Joback Method
dvisc	0.0001978	Paxs	612.21	Joback Method

Sources

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=U352913&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

cp_g:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
g_f:	Standard Gibbs free energy of formation
h_f:	Enthalpy of formation at standard conditions
h_{fus}:	Enthalpy of fusion at standard conditions
h_{vap}:	Enthalpy of vaporization at standard conditions
log₁₀w_s:	Log ₁₀ of Water solubility in mol/l
log_p:	Octanol/Water partition coefficient
mc_{vol}:	McGowan's characteristic volume
pc:	Critical Pressure
rin_{pol}:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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