

# p-acetoxy-acetanilide

<b>Inchi:</b>	InChI=1S/C10H11NO3/c1-7(12)11-9-3-5-10(6-4-9)14-8(2)13/h3-6H,1-2H3,(H,11,12)
<b>InchiKey:</b>	UJAOSPFULOFZRR-UHFFFAOYSA-N
<b>Formula:</b>	C10H11NO3
<b>SMILES:</b>	CC(=O)Nc1ccc(OC(C)=O)cc1
<b>Mol. weight [g/mol]:</b>	193.20

## Physical Properties

Property code	Value	Unit	Source
gf	-137.35	kJ/mol	Joback Method
hf	-328.58	kJ/mol	Joback Method
hfus	24.79	kJ/mol	Joback Method
hvap	63.13	kJ/mol	Joback Method
log10ws	-1.91		Aqueous Solubility Prediction Method
logp	1.570		Crippen Method
mcvol	146.990	ml/mol	McGowan Method
pc	3302.95	kPa	Joback Method
tb	640.19	K	Joback Method
tc	860.95	K	Joback Method
tf	416.15	K	Joback Method
vc	0.552	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	362.17	J/molxK	640.19	Joback Method
cpg	374.16	J/molxK	676.98	Joback Method
cpg	385.36	J/molxK	713.78	Joback Method
cpg	395.79	J/molxK	750.57	Joback Method
cpg	405.45	J/molxK	787.37	Joback Method
cpg	414.37	J/molxK	824.16	Joback Method
cpg	422.55	J/molxK	860.95	Joback Method

# Sources

<b>McGowan Method:</b>	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</a>
<b>Joback Method:</b>	<a href="https://en.wikipedia.org/wiki/Joback_method">https://en.wikipedia.org/wiki/Joback_method</a>
<b>Aqueous Solubility Prediction Method:</b>	<a href="http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa">http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa</a>

# Legend

<b>cpg:</b>	Ideal gas heat capacity
<b>gf:</b>	Standard Gibbs free energy of formation
<b>hf:</b>	Enthalpy of formation at standard conditions
<b>hfus:</b>	Enthalpy of fusion at standard conditions
<b>hvap:</b>	Enthalpy of vaporization at standard conditions
<b>log10ws:</b>	Log10 of Water solubility in mol/l
<b>logp:</b>	Octanol/Water partition coefficient
<b>mcvol:</b>	McGowan's characteristic volume
<b>pc:</b>	Critical Pressure
<b>tb:</b>	Normal Boiling Point Temperature
<b>tc:</b>	Critical Temperature
<b>tf:</b>	Normal melting (fusion) point
<b>vc:</b>	Critical Volume

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