

# P-Hydroxyhippuric acid, methyl ester

<b>Inchi:</b>	InChI=1S/C10H11NO4/c1-15-9(13)6-11-10(14)7-2-4-8(12)5-3-7/h2-5,12H,6H2,1H3,(H,1
<b>InchiKey:</b>	RNPKFTDQICBOQY-UHFFFAOYSA-N
<b>Formula:</b>	C10H11NO4
<b>SMILES:</b>	COC(=O)CNC(=O)c1ccc(O)cc1
<b>Mol. weight [g/mol]:</b>	209.20

## Physical Properties

Property code	Value	Unit	Source
gf	-282.34	kJ/mol	Joback Method
hf	-494.42	kJ/mol	Joback Method
hfus	30.96	kJ/mol	Joback Method
hvap	75.48	kJ/mol	Joback Method
log10ws	-1.06		Crippen Method
logp	0.295		Crippen Method
mcvol	152.860	ml/mol	McGowan Method
pc	4026.13	kPa	Joback Method
rinpol	2027.00		NIST Webbook
rinpol	2027.00		NIST Webbook
tb	715.83	K	Joback Method
tc	943.94	K	Joback Method
tf	515.35	K	Joback Method
vc	0.518	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	408.23	J/mol×K	715.83	Joback Method
cpg	418.75	J/mol×K	753.85	Joback Method
cpg	428.55	J/mol×K	791.87	Joback Method
cpg	437.71	J/mol×K	829.89	Joback Method
cpg	446.29	J/mol×K	867.91	Joback Method
cpg	454.36	J/mol×K	905.93	Joback Method
cpg	461.98	J/mol×K	943.94	Joback Method

# Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=R245655&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R245655&amp;Units=SI</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>Crippen Method:</b>	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>
<b>Joback Method:</b>	<a href="https://en.wikipedia.org/wiki/Joback_method">https://en.wikipedia.org/wiki/Joback_method</a>
<b>McGowan Method:</b>	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</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>hvp:</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>rinp:</b>	Non-polar retention indices
<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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