

# «alpha»-Methylcinnamic acid

<b>Other names:</b>	2-Propenoic acid, 2-methyl-3-phenyl-Cinnamic acid, «alpha»-methyl-2-Methyl-3-phenyl-2-propenoic acid
<b>Inchi:</b>	InChI=1S/C10H10O2/c1-8(10(11)12)7-9-5-3-2-4-6-9/h2-7H,1H3,(H,11,12)/b8-7+
<b>InchiKey:</b>	XNCRUNXWPDJHGKV-BQYQJAHWSA-N
<b>Formula:</b>	C10H10O2
<b>SMILES:</b>	CC(=Cc1ccccc1)C(=O)O
<b>Mol. weight [g/mol]:</b>	162.19
<b>CAS:</b>	1199-77-5

## Physical Properties

Property code	Value	Unit	Source
gf	-48.34	kJ/mol	Joback Method
hf	-170.58	kJ/mol	Joback Method
hfus	20.28	kJ/mol	Joback Method
hvap	63.59	kJ/mol	Joback Method
log10ws	-2.23		Crippen Method
logp	2.174		Crippen Method
mcvol	131.140	ml/mol	McGowan Method
pc	3740.80	kPa	Joback Method
tb	604.97	K	Joback Method
tc	817.08	K	Joback Method
tf	320.59	K	Joback Method
vc	0.493	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	306.62	J/mol×K	604.97	Joback Method
cpg	317.42	J/mol×K	640.32	Joback Method
cpg	327.48	J/mol×K	675.67	Joback Method
cpg	336.84	J/mol×K	711.02	Joback Method
cpg	345.56	J/mol×K	746.37	Joback Method
cpg	353.69	J/mol×K	781.72	Joback Method

cpg	361.26	J/mol×K	817.08	Joback Method
hvapt	78.50	kJ/mol	479.50	NIST Webbook

## Sources

<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>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C1199775&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C1199775&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307l">http://pubs.acs.org/doi/abs/10.1021/ci990307l</a>
<b>Crippen Method:</b>	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</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>hvapt:</b>	Enthalpy of vaporization at a given temperature
<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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