

# 3,5-(CH<sub>3</sub>)=C<sub>6</sub>H<sub>3</sub>-COCH<sub>3</sub>

<b>Inchi:</b>	InChI=1S/C10H12O/c1-7-4-8(2)6-10(5-7)9(3)11/h4-6H,1-3H3
<b>InchiKey:</b>	BKIHFLZLJJUNKMZ-UHFFFAOYSA-N
<b>Formula:</b>	C10H12O
<b>SMILES:</b>	CC(=O)c1cc(C)cc(C)c1
<b>Mol. weight [g/mol]:</b>	148.20
<b>CAS:</b>	5379-16-8

## Physical Properties

Property code	Value	Unit	Source
affp	876.00	kJ/mol	NIST Webbook
basg	844.20	kJ/mol	NIST Webbook
gf	-2.45	kJ/mol	Joback Method
hf	-148.72	kJ/mol	Joback Method
hfus	16.52	kJ/mol	Joback Method
hvap	48.20	kJ/mol	Joback Method
log10ws	-3.08		Crippen Method
logp	2.506		Crippen Method
mcvol	129.570	ml/mol	McGowan Method
pc	3038.96	kPa	Joback Method
tb	518.71	K	Joback Method
tc	735.99	K	Joback Method
tf	303.85	K	Joback Method
vc	0.493	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	276.59	J/molxK	518.71	Joback Method
cpg	335.57	J/molxK	699.77	Joback Method
cpg	325.13	J/molxK	663.56	Joback Method
cpg	314.04	J/molxK	627.35	Joback Method
cpg	302.26	J/molxK	591.14	Joback Method
cpg	289.78	J/molxK	554.92	Joback Method
cpg	345.38	J/molxK	735.99	Joback Method

dvisc	0.0002423	Paxs	518.71	Joback Method
dvisc	0.0002973	Paxs	482.90	Joback Method
dvisc	0.0003768	Paxs	447.09	Joback Method
dvisc	0.0004977	Paxs	411.28	Joback Method
dvisc	0.0006932	Paxs	375.47	Joback Method
dvisc	0.0010355	Paxs	339.66	Joback Method
dvisc	0.0017002	Paxs	303.85	Joback Method

## Sources

<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>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C5379168&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C5379168&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>

## Legend

<b>affp:</b>	Proton affinity
<b>basg:</b>	Gas basicity
<b>cpg:</b>	Ideal gas heat capacity
<b>dvisc:</b>	Dynamic viscosity
<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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