

# 3-Methylcatechol, diacetate

<b>Inchi:</b>	InChI=1S/C11H12O4/c1-7-5-4-6-10(14-8(2)12)11(7)15-9(3)13/h4-6H,1-3H3
<b>InchiKey:</b>	WSDQZFOBIKMDJE-UHFFFAOYSA-N
<b>Formula:</b>	C11H12O4
<b>SMILES:</b>	CC(=O)Oc1cccc(C)c1OC(C)=O
<b>Mol. weight [g/mol]:</b>	208.21

## Physical Properties

Property code	Value	Unit	Source
gf	-332.95	kJ/mol	Joback Method
hf	-546.38	kJ/mol	Joback Method
hfus	23.08	kJ/mol	Joback Method
hvap	61.99	kJ/mol	Joback Method
log10ws	-2.57		Crippen Method
logp	1.846		Crippen Method
mcvol	156.970	ml/mol	McGowan Method
pc	2826.33	kPa	Joback Method
rinpol	1452.50		NIST Webbook
tb	640.30	K	Joback Method
tc	856.49	K	Joback Method
tf	409.51	K	Joback Method
vc	0.592	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	385.86	J/mol×K	640.30	Joback Method
cpg	398.36	J/mol×K	676.33	Joback Method
cpg	410.14	J/mol×K	712.36	Joback Method
cpg	421.20	J/mol×K	748.40	Joback Method
cpg	431.51	J/mol×K	784.43	Joback Method
cpg	441.07	J/mol×K	820.46	Joback Method
cpg	449.88	J/mol×K	856.49	Joback Method
dvisc	0.0009633	Paxs	409.51	Joback Method
dvisc	0.0006315	Paxs	447.97	Joback Method

dvisc	0.0004426	Paxs	486.44	Joback Method
dvisc	0.0003268	Paxs	524.90	Joback Method
dvisc	0.0002515	Paxs	563.37	Joback Method
dvisc	0.0002001	Paxs	601.84	Joback Method
dvisc	0.0001637	Paxs	640.30	Joback Method

## 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=U352789&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U352789&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.cheméo.com/doc/models/crippen_log10ws">https://www.cheméo.com/doc/models/crippen_log10ws</a>

## Legend

<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>rinpol:</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

Latest version available from:

<https://www.cheméo.com/cid/54-868-9/3-Methylcatechol-diacetate.pdf>

Generated by Cheméo on 2025-12-05 16:30:36.881632071 +0000 UTC m=+4700434.411672725.

Cheméo (<https://www.cheméo.com>) is the biggest free database of chemical and physical data for the process industry.