

# Cyclopropanecarboxylic acid, 3-methylphenyl ester

Inchi:	InChI=1S/C11H12O2/c1-8-3-2-4-10(7-8)13-11(12)9-5-6-9/h2-4,7,9H,5-6H2,1H3
InchiKey:	WGLQWJBSGPCLSV-UHFFFAOYSA-N
Formula:	C11H12O2
SMILES:	<chem>Cc1cccc(OC(=O)C2CC2)c1</chem>
Mol. weight [g/mol]:	176.21

## Physical Properties

Property code	Value	Unit	Source
gf	-28.65	kJ/mol	Joback Method
hf	-217.31	kJ/mol	Joback Method
hfus	18.82	kJ/mol	Joback Method
hvap	52.09	kJ/mol	Joback Method
log10ws	-2.75		Crippen Method
logp	2.310		Crippen Method
mvol	138.670	ml/mol	McGowan Method
pc	3149.09	kPa	Joback Method
rinpol	1382.00		NIST Webbook
rinpol	1382.00		NIST Webbook
tb	565.77	K	Joback Method
tc	791.94	K	Joback Method
tf	342.77	K	Joback Method
vc	0.524	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	331.55	J/molxK	565.77	Joback Method
cpg	396.47	J/molxK	754.25	Joback Method
cpg	385.26	J/molxK	716.55	Joback Method
cpg	373.21	J/molxK	678.86	Joback Method
cpg	360.28	J/molxK	641.16	Joback Method
cpg	346.41	J/molxK	603.47	Joback Method
cpg	406.89	J/molxK	791.94	Joback Method
dvisc	0.0004407	Paxs	565.77	Joback Method

dvisc	0.0005103	Paxs	528.60	Joback Method
dvisc	0.0006042	Paxs	491.44	Joback Method
dvisc	0.0007355	Paxs	454.27	Joback Method
dvisc	0.0009272	Paxs	417.10	Joback Method
dvisc	0.0012230	Paxs	379.94	Joback Method
dvisc	0.0017132	Paxs	342.77	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=U307521&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U307521&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>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

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