

# Cyclopropanecarboxylic acid, trans-2-phenyl-, tridec-6-yl ester

<b>Inchi:</b>	InChI=1S/C23H36O2/c1-3-5-7-8-13-17-20(16-10-6-4-2)25-23(24)22-18-21(22)19-14-11-9
<b>InchiKey:</b>	MJMJRYNFEKYKJW-UHFFFAOYSA-N
<b>Formula:</b>	C23H36O2
<b>SMILES:</b>	CCCCCCCC(CCCCC)OC(=O)C1CC1c1ccccc1
<b>Mol. weight [g/mol]:</b>	344.53

## Physical Properties

Property code	Value	Unit	Source
gf	71.87	kJ/mol	Joback Method
hf	-479.14	kJ/mol	Joback Method
hfus	47.84	kJ/mol	Joback Method
hvap	77.44	kJ/mol	Joback Method
log10ws	-7.14		Crippen Method
logp	6.643		Crippen Method
mvol	307.750	ml/mol	McGowan Method
pc	1153.78	kPa	Joback Method
rinpol	2439.00		NIST Webbook
rinpol	2439.00		NIST Webbook
tb	830.24	K	Joback Method
tc	1030.19	K	Joback Method
tf	446.25	K	Joback Method
vc	1.190	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	993.90	J/molxK	830.24	Joback Method
cpg	1013.46	J/molxK	863.57	Joback Method
cpg	1031.82	J/molxK	896.89	Joback Method
cpg	1049.07	J/molxK	930.22	Joback Method
cpg	1065.26	J/molxK	963.54	Joback Method
cpg	1080.47	J/molxK	996.87	Joback Method
cpg	1094.75	J/molxK	1030.19	Joback Method
dvisc	0.0016481	Paxs	446.25	Joback Method

dvisc	0.0009001	Paxs	510.25	Joback Method
dvisc	0.0005625	Paxs	574.25	Joback Method
dvisc	0.0003863	Paxs	638.25	Joback Method
dvisc	0.0002841	Paxs	702.24	Joback Method
dvisc	0.0002199	Paxs	766.24	Joback Method
dvisc	0.0001771	Paxs	830.24	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=U406253&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U406253&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>cp<sub>g</sub>:</b>	Ideal gas heat capacity
<b>dvisc:</b>	Dynamic viscosity
<b>g<sub>f</sub>:</b>	Standard Gibbs free energy of formation
<b>h<sub>f</sub>:</b>	Enthalpy of formation at standard conditions
<b>h<sub>fus</sub>:</b>	Enthalpy of fusion at standard conditions
<b>h<sub>vap</sub>:</b>	Enthalpy of vaporization at standard conditions
<b>log<sub>10</sub>w<sub>s</sub>:</b>	Log <sub>10</sub> of Water solubility in mol/l
<b>log<sub>p</sub>:</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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