

# Cyclohexanecarboxylic acid, 3,5-dimethylphenyl ester

Inchi:	InChI=1S/C15H20O2/c1-11-8-12(2)10-14(9-11)17-15(16)13-6-4-3-5-7-13/h8-10,13H,3-7H
InchiKey:	ZJPBGWIGOQJVBM-UHFFFAOYSA-N
Formula:	C15H20O2
SMILES:	<chem>Cc1cc(C)cc(OC(=O)C2CCCCC2)c1</chem>
Mol. weight [g/mol]:	232.32

## Physical Properties

Property code	Value	Unit	Source
gf	-40.90	kJ/mol	Joback Method
hf	-329.82	kJ/mol	Joback Method
hfus	22.49	kJ/mol	Joback Method
hvap	62.17	kJ/mol	Joback Method
log10ws	-4.48		Crippen Method
logp	3.789		Crippen Method
mcvol	195.030	ml/mol	McGowan Method
pc	2254.67	kPa	Joback Method
rinpol	1796.00		NIST Webbook
rinpol	1796.00		NIST Webbook
tb	675.08	K	Joback Method
tc	907.35	K	Joback Method
tf	389.81	K	Joback Method
vc	0.725	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	538.40	J/molxK	675.08	Joback Method
cpg	557.78	J/molxK	713.79	Joback Method
cpg	575.80	J/molxK	752.50	Joback Method
cpg	592.51	J/molxK	791.21	Joback Method
cpg	607.93	J/molxK	829.93	Joback Method
cpg	622.09	J/molxK	868.64	Joback Method
cpg	635.02	J/molxK	907.35	Joback Method
dvisc	0.0014577	Paxs	389.81	Joback Method

dvisc	0.0008012	Paxs	437.36	Joback Method
dvisc	0.0004952	Paxs	484.90	Joback Method
dvisc	0.0003335	Paxs	532.45	Joback Method
dvisc	0.0002397	Paxs	579.99	Joback Method
dvisc	0.0001811	Paxs	627.54	Joback Method
dvisc	0.0001423	Paxs	675.08	Joback Method

## Sources

<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=U307704&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U307704&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.cheméo.com/doc/models/crippen_log10ws">https://www.cheméo.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>

## 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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