

# Cyclohexanecarboxylic acid, tridecyl ester

**Inchi:** InChI=1S/C20H38O2/c1-2-3-4-5-6-7-8-9-10-11-15-18-22-20(21)19-16-13-12-14-17-19/h1-19,21-22H,20H2  
**InchiKey:** NYSRVOQLCGJDRW-UHFFFAOYSA-N  
**Formula:** C20H38O2  
**SMILES:** CCCCCCCCCCCCCOC(=O)C1CCCCC1  
**Mol. weight [g/mol]:** 310.51

## Physical Properties

Property code	Value	Unit	Source
gf	-91.95	kJ/mol	Joback Method
hf	-646.61	kJ/mol	Joback Method
hfus	42.18	kJ/mol	Joback Method
hvap	69.70	kJ/mol	Joback Method
log10ws	-6.71		Crippen Method
logp	6.421		Crippen Method
mcvol	289.240	ml/mol	McGowan Method
pc	1199.79	kPa	Joback Method
rinsol	2240.00		NIST Webbook
tb	752.84	K	Joback Method
tc	939.55	K	Joback Method
tf	394.70	K	Joback Method
vc	1.113	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	906.57	J/molxK	752.84	Joback Method
cpg	927.73	J/molxK	783.96	Joback Method
cpg	947.70	J/molxK	815.08	Joback Method
cpg	966.52	J/molxK	846.19	Joback Method
cpg	984.23	J/molxK	877.31	Joback Method
cpg	1000.85	J/molxK	908.43	Joback Method
cpg	1016.41	J/molxK	939.55	Joback Method
dvisc	0.0019497	Paxs	394.70	Joback Method
dvisc	0.0007974	Paxs	454.39	Joback Method

dvisc	0.0004014	Paxs	514.08	Joback Method
dvisc	0.0002331	Paxs	573.77	Joback Method
dvisc	0.0001499	Paxs	633.46	Joback Method
dvisc	0.0001041	Paxs	693.15	Joback Method
dvisc	0.0000765	Paxs	752.84	Joback Method

## Sources

<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.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=U279541&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U279541&amp;Units=SI</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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