

# Cyclohexanecarboxylic acid, 4-methoxy-, tridecyl ester

Inchi:	InChI=1S/C21H40O3/c1-3-4-5-6-7-8-9-10-11-12-13-18-24-21(22)19-14-16-20(23-2)17-15
InchiKey:	LIKUENJUJVSIDS-UHFFFAOYSA-N
Formula:	C21H40O3
SMILES:	CCCCCCCCCCCCOC(=O)C1CCC(OC)CC1
Mol. weight [g/mol]:	340.54

## Physical Properties

Property code	Value	Unit	Source
gf	-196.24	kJ/mol	Joback Method
hf	-819.81	kJ/mol	Joback Method
hfus	47.03	kJ/mol	Joback Method
hvap	74.03	kJ/mol	Joback Method
log10ws	-6.33		Crippen Method
logp	6.046		Crippen Method
mvol	309.200	ml/mol	McGowan Method
pc	1087.06	kPa	Joback Method
rinpol	2468.00		NIST Webbook
rinpol	2468.00		NIST Webbook
tb	793.47	K	Joback Method
tc	981.49	K	Joback Method
tf	423.96	K	Joback Method
vc	1.185	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1003.70	J/molxK	793.47	Joback Method
cpg	1024.92	J/molxK	824.81	Joback Method
cpg	1044.87	J/molxK	856.14	Joback Method
cpg	1063.54	J/molxK	887.48	Joback Method
cpg	1080.98	J/molxK	918.82	Joback Method
cpg	1097.19	J/molxK	950.15	Joback Method
cpg	1112.19	J/molxK	981.49	Joback Method
dvisc	0.0011736	Paxs	423.96	Joback Method

dvisc	0.0005304	Paxs	485.54	Joback Method
dvisc	0.0002866	Paxs	547.13	Joback Method
dvisc	0.0001754	Paxs	608.72	Joback Method
dvisc	0.0001175	Paxs	670.30	Joback Method
dvisc	0.0000842	Paxs	731.88	Joback Method
dvisc	0.0000635	Paxs	793.47	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=U406201&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U406201&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>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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