

# Cyclohexane,1-(1,1-dimethylethyl)-3-methoxy-4-m

<b>Inchi:</b>	InChI=1S/C12H22O/c1-9-6-7-10(12(2,3)4)8-11(9)13-5/h10-11H,1,6-8H2,2-5H3/t10-,11-/m
<b>InchiKey:</b>	DUVGSEXMTVWEHI-GHMZBOCLSA-N
<b>Formula:</b>	C12H22O
<b>SMILES:</b>	C=C1CCC(C(C)(C)C)CC1OC
<b>Mol. weight [g/mol]:</b>	182.30
<b>CAS:</b>	68211-39-2

## Physical Properties

Property code	Value	Unit	Source
gf	17.82	kJ/mol	Joback Method
hf	-313.76	kJ/mol	Joback Method
hfus	12.36	kJ/mol	Joback Method
hvap	43.70	kJ/mol	Joback Method
ie	8.97 ± 0.02	eV	NIST Webbook
ie	8.97 ± 0.05	eV	NIST Webbook
log10ws	-3.31		Crippen Method
logp	3.404		Crippen Method
mcvol	170.650	ml/mol	McGowan Method
pc	2110.00	kPa	Joback Method
tb	507.19	K	Joback Method
tc	711.61	K	Joback Method
tf	266.47	K	Joback Method
vc	0.630	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	409.35	J/molxK	507.19	Joback Method
cpg	503.65	J/molxK	677.54	Joback Method
cpg	486.83	J/molxK	643.47	Joback Method
cpg	469.01	J/molxK	609.40	Joback Method
cpg	450.17	J/molxK	575.33	Joback Method
cpg	430.30	J/molxK	541.26	Joback Method
cpg	519.50	J/molxK	711.61	Joback Method

dvisc	0.0002119	Paxs	507.19	Joback Method
dvisc	0.0002745	Paxs	467.07	Joback Method
dvisc	0.0003732	Paxs	426.95	Joback Method
dvisc	0.0005408	Paxs	386.83	Joback Method
dvisc	0.0008540	Paxs	346.71	Joback Method
dvisc	0.0015197	Paxs	306.59	Joback Method
dvisc	0.0032171	Paxs	266.47	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=C68211392&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C68211392&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>ie:</b>	Ionization energy
<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>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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