

# Tricyclo[4.3.1.1(2,5)]undecane, 10-methoxy-, stereoisomer

**Inchi:** InChI=1S/C12H20O/c1-13-12-10-3-2-4-11(12)9-6-5-8(10)7-9/h8-12H,2-7H2,1H3  
**InchiKey:** FZLYZEQLJWOGIF-UHFFFAOYSA-N  
**Formula:** C12H20O  
**SMILES:** COC1C2CCCC1C1CCC2C1  
**Mol. weight [g/mol]:** 180.29  
**CAS:** 85538-50-7

## Physical Properties

Property code	Value	Unit	Source
gf	87.79	kJ/mol	Joback Method
hf	-257.83	kJ/mol	Joback Method
hfus	20.37	kJ/mol	Joback Method
hvap	44.18	kJ/mol	Joback Method
ie	9.10	eV	NIST Webbook
ie	8.50	eV	NIST Webbook
log10ws	-2.76		Crippen Method
logp	2.848		Crippen Method
mcvol	153.230	ml/mol	McGowan Method
pc	2467.81	kPa	Joback Method
tb	515.80	K	Joback Method
tc	729.04	K	Joback Method
tf	285.53	K	Joback Method
vc	0.579	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	398.11	J/molxK	515.80	Joback Method
cpg	420.91	J/molxK	551.34	Joback Method
cpg	442.33	J/molxK	586.88	Joback Method
cpg	462.43	J/molxK	622.42	Joback Method
cpg	481.29	J/molxK	657.96	Joback Method
cpg	498.97	J/molxK	693.50	Joback Method
cpg	515.56	J/molxK	729.04	Joback Method

dvisc	0.0010770	Paxs	285.53	Joback Method
dvisc	0.0011013	Paxs	323.91	Joback Method
dvisc	0.0011208	Paxs	362.29	Joback Method
dvisc	0.0011369	Paxs	400.66	Joback Method
dvisc	0.0011503	Paxs	439.04	Joback Method
dvisc	0.0011616	Paxs	477.42	Joback Method
dvisc	0.0011714	Paxs	515.80	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=C85538507&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C85538507&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>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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