

# 3,3'-(2,2,4,4-Tetramethyl-1,3-cyclobutylendioxy)oc

<b>Inchi:</b>	InChI=1S/C14H22N2O2/c1-13(2)11(17-9-5-7-15)14(3,4)12(13)18-10-6-8-16/h11-12H,5-6
<b>InchiKey:</b>	PNKHZYPFJHQBFC-UHFFFAOYSA-N
<b>Formula:</b>	C14H22N2O2
<b>SMILES:</b>	CC1(C)C(OCCC#N)C(C)(C)C1OCCC#N
<b>Mol. weight [g/mol]:</b>	250.34
<b>CAS:</b>	1731-46-0

## Physical Properties

Property code	Value	Unit	Source
gf	137.90	kJ/mol	Joback Method
hf	-230.87	kJ/mol	Joback Method
hfus	24.06	kJ/mol	Joback Method
hvap	69.39	kJ/mol	Joback Method
log10ws	-3.23		Crippen Method
logp	2.650		Crippen Method
mcvol	211.760	ml/mol	McGowan Method
pc	1600.00	kPa	Joback Method
tb	766.20	K	Joback Method
tc	979.02	K	Joback Method
tf	471.48	K	Joback Method
vc	0.850	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	637.52	J/molxK	766.20	Joback Method
cpg	653.89	J/molxK	801.67	Joback Method
cpg	670.13	J/molxK	837.14	Joback Method
cpg	686.41	J/molxK	872.61	Joback Method
cpg	702.89	J/molxK	908.08	Joback Method
cpg	719.74	J/molxK	943.55	Joback Method
cpg	737.12	J/molxK	979.02	Joback Method

# Sources

<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307I">http://pubs.acs.org/doi/abs/10.1021/ci990307I</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=C1731460&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C1731460&amp;Units=SI</a>

# Legend

<b>cpg:</b>	Ideal gas heat capacity
<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>mccvol:</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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