

# Cyclohexane, 1,1'-(1-methyl-1,3-propanediyl)bis-

Other names:	1,3-Dicyclohexylbutane
Inchi:	InChI=1S/C16H30/c1-14(16-10-6-3-7-11-16)12-13-15-8-4-2-5-9-15/h14-16H,2-13H2,1H3
InchiKey:	QYUDFQUDLLTCAA-UHFFFAOYSA-N
Formula:	C16H30
SMILES:	CC(CCC1CCCCC1)C1CCCCC1
Mol. weight [g/mol]:	222.41
CAS:	41851-35-8

## Physical Properties

Property code	Value	Unit	Source
chl	-10220.00	kJ/mol	NIST Webbook
gf	130.30	kJ/mol	Joback Method
hf	-270.21	kJ/mol	Joback Method
hfus	17.34	kJ/mol	Joback Method
hvap	51.68	kJ/mol	Joback Method
log10ws	-5.58		Crippen Method
logp	5.563		Crippen Method
mcvol	214.580	ml/mol	McGowan Method
pc	1832.54	kPa	Joback Method
tb	576.34 ± 0.30	K	NIST Webbook
tc	824.40	K	Joback Method
tf	269.84	K	Joback Method
vc	0.791	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	601.49	J/mol×K	604.14	Joback Method
cpg	741.10	J/mol×K	824.40	Joback Method
cpg	721.69	J/mol×K	787.69	Joback Method
cpg	700.82	J/mol×K	750.98	Joback Method
cpg	678.42	J/mol×K	714.27	Joback Method
cpg	654.44	J/mol×K	677.56	Joback Method
cpg	628.82	J/mol×K	640.85	Joback Method

cpl	359.40	J/molxK	313.00	NIST Webbook
dvisc	0.0001627	Paxs	604.14	Joback Method
dvisc	0.0002317	Paxs	548.42	Joback Method
dvisc	0.0003575	Paxs	492.71	Joback Method
dvisc	0.0006161	Paxs	436.99	Joback Method
dvisc	0.0012448	Paxs	381.27	Joback Method
dvisc	0.0031999	Paxs	325.56	Joback Method
dvisc	0.0121478	Paxs	269.84	Joback Method

## Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.39762e+01
Coeff. B	-4.44468e+03
Coeff. C	-1.01373e+02
Temperature range (K), min.	426.07
Temperature range (K), max.	614.34

## Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C41851358&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C41851358&amp;Units=SI</a>
<b>The Yaws Handbook of Vapor Pressure:</b>	<a href="https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure">https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure</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>
<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>

## Legend

<b>chl:</b>	Standard liquid enthalpy of combustion
<b>cpg:</b>	Ideal gas heat capacity
<b>cpl:</b>	Liquid phase 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>pvap:</b>	Vapor 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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