

# 1,2-Cyclohexanedicarboxylic acid, butyl furfuryl ester

Inchi:	InChI=1S/C17H28O5/c1-2-3-10-21-16(18)14-8-4-5-9-15(14)17(19)22-12-13-7-6-11-20-13
InchiKey:	WEXOBQVQMZSOEI-UHFFFAOYSA-N
Formula:	C17H28O5
SMILES:	CCCCOC(=O)C1CCCCC1C(=O)OCC1CCCO1
Mol. weight [g/mol]:	312.40

## Physical Properties

Property code	Value	Unit	Source
gf	-408.41	kJ/mol	Joback Method
hf	-921.35	kJ/mol	Joback Method
hfus	40.18	kJ/mol	Joback Method
hvap	76.64	kJ/mol	Joback Method
log10ws	-3.17		Crippen Method
logp	2.858		Crippen Method
mcvol	249.420	ml/mol	McGowan Method
pc	1714.61	kPa	Joback Method
rinpol	2218.00		NIST Webbook
rinpol	2218.00		NIST Webbook
tb	798.05	K	Joback Method
tc	1011.49	K	Joback Method
tf	466.28	K	Joback Method
vc	0.929	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	816.88	J/molxK	798.05	Joback Method
cpg	836.02	J/molxK	833.62	Joback Method
cpg	853.65	J/molxK	869.20	Joback Method
cpg	869.81	J/molxK	904.77	Joback Method
cpg	884.52	J/molxK	940.34	Joback Method
cpg	897.79	J/molxK	975.92	Joback Method
cpg	909.64	J/molxK	1011.49	Joback Method
dvisc	0.0014714	Paxs	466.28	Joback Method

dvisc	0.0008033	Paxs	521.57	Joback Method
dvisc	0.0004925	Paxs	576.87	Joback Method
dvisc	0.0003289	Paxs	632.16	Joback Method
dvisc	0.0002344	Paxs	687.46	Joback Method
dvisc	0.0001757	Paxs	742.75	Joback Method
dvisc	0.0001371	Paxs	798.05	Joback Method

## Sources

<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=U339897&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U339897&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>
<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>

## 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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