

# 1,2-Cyclohexanedicarboxylic acid, butyl hexyl ester

Inchi:	InChI=1S/C18H32O4/c1-3-5-7-10-14-22-18(20)16-12-9-8-11-15(16)17(19)21-13-6-4-2/h
InchiKey:	JZDKKCSTIGLISW-UHFFFAOYSA-N
Formula:	C18H32O4
SMILES:	CCCCCOC(=O)C1CCCCC1C(=O)OCCCC
Mol. weight [g/mol]:	312.44

## Physical Properties

Property code	Value	Unit	Source
gf	-350.42	kJ/mol	Joback Method
hf	-870.47	kJ/mol	Joback Method
hfus	40.86	kJ/mol	Joback Method
hvap	74.09	kJ/mol	Joback Method
log10ws	-4.49		Crippen Method
logp	4.260		Crippen Method
mvol	268.500	ml/mol	McGowan Method
pc	1390.22	kPa	Joback Method
rinpol	2114.00		NIST Webbook
rinpol	2114.00		NIST Webbook
tb	778.70	K	Joback Method
tc	973.21	K	Joback Method
tf	440.08	K	Joback Method
vc	1.024	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	848.78	J/molxK	778.70	Joback Method
cpg	931.83	J/molxK	940.79	Joback Method
cpg	917.63	J/molxK	908.37	Joback Method
cpg	902.23	J/molxK	875.95	Joback Method
cpg	885.63	J/molxK	843.54	Joback Method
cpg	867.82	J/molxK	811.12	Joback Method
cpg	944.86	J/molxK	973.21	Joback Method
dvisc	0.0000926	Paxs	778.70	Joback Method

dvisc	0.0001205	Paxs	722.26	Joback Method
dvisc	0.0001638	Paxs	665.83	Joback Method
dvisc	0.0002358	Paxs	609.39	Joback Method
dvisc	0.0003655	Paxs	552.95	Joback Method
dvisc	0.0006262	Paxs	496.52	Joback Method
dvisc	0.0012314	Paxs	440.08	Joback Method

## Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=U339409&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U339409&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>
<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>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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