

# 1,2-Cyclohexanedicarboxylic acid, isobutyl 2-methylpent-3-yl ester

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

## Physical Properties

Property code	Value	Unit	Source
gf	-357.74	kJ/mol	Joback Method
hf	-886.31	kJ/mol	Joback Method
hfus	30.29	kJ/mol	Joback Method
hvap	72.93	kJ/mol	Joback Method
log10ws	-4.12		Crippen Method
logp	3.970		Crippen Method
mvol	268.500	ml/mol	McGowan Method
pc	1415.44	kPa	Joback Method
rinpol	2032.00		NIST Webbook
rinpol	2032.00		NIST Webbook
tb	777.38	K	Joback Method
tc	979.06	K	Joback Method
tf	395.08	K	Joback Method
vc	1.006	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	850.23	J/molxK	777.38	Joback Method
cpg	935.67	J/molxK	945.45	Joback Method
cpg	921.23	J/molxK	911.83	Joback Method
cpg	905.48	J/molxK	878.22	Joback Method
cpg	888.40	J/molxK	844.61	Joback Method
cpg	869.99	J/molxK	810.99	Joback Method
cpg	948.82	J/molxK	979.06	Joback Method
dvisc	0.0000721	Paxs	777.38	Joback Method

dvisc	0.0000987	Paxs	713.66	Joback Method
dvisc	0.0001436	Paxs	649.95	Joback Method
dvisc	0.0002268	Paxs	586.23	Joback Method
dvisc	0.0004004	Paxs	522.51	Joback Method
dvisc	0.0008276	Paxs	458.80	Joback Method
dvisc	0.0021620	Paxs	395.08	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=U339441&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U339441&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.cheméo.com/doc/models/crippen_log10ws">https://www.cheméo.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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