

# 1,2-Cyclohexanedicarboxylic acid, isobutyl isopropyl ester

Inchi:	InChI=1S/C15H26O4/c1-10(2)9-18-14(16)12-7-5-6-8-13(12)15(17)19-11(3)4/h10-13H,5-9
InchiKey:	JLXUJVVDYOFHHMU-UHFFFAOYSA-N
Formula:	C15H26O4
SMILES:	CC(C)COC(=O)C1CCCCC1C(=O)OC(C)C
Mol. weight [g/mol]:	270.36

## Physical Properties

Property code	Value	Unit	Source
gf	-380.56	kJ/mol	Joback Method
hf	-819.11	kJ/mol	Joback Method
hfus	26.04	kJ/mol	Joback Method
hvap	66.64	kJ/mol	Joback Method
log10ws	-3.11		Crippen Method
logp	2.944		Crippen Method
mvol	226.230	ml/mol	McGowan Method
pc	1768.38	kPa	Joback Method
rinpol	1905.00		NIST Webbook
tb	709.18	K	Joback Method
tc	913.13	K	Joback Method
tf	376.27	K	Joback Method
vc	0.844	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	675.17	J/molxK	709.18	Joback Method
cpg	759.27	J/molxK	879.14	Joback Method
cpg	744.83	J/molxK	845.15	Joback Method
cpg	729.21	J/molxK	811.16	Joback Method
cpg	712.39	J/molxK	777.16	Joback Method
cpg	694.38	J/molxK	743.17	Joback Method
cpg	772.52	J/molxK	913.13	Joback Method
dvisc	0.0001157	Paxs	709.18	Joback Method
dvisc	0.0001544	Paxs	653.69	Joback Method

dvisc	0.0002174	Paxs	598.21	Joback Method
dvisc	0.0003283	Paxs	542.72	Joback Method
dvisc	0.0005445	Paxs	487.24	Joback Method
dvisc	0.0010286	Paxs	431.75	Joback Method
dvisc	0.0023439	Paxs	376.27	Joback Method

## Sources

<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>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=U339636&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U339636&amp;Units=SI</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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