

# 1,2-Cyclohexanedicarboxylic acid, hexyl isobutyl ester

Inchi:	InChI=1S/C18H32O4/c1-4-5-6-9-12-21-17(19)15-10-7-8-11-16(15)18(20)22-13-14(2)3/h1
InchiKey:	DRNQUQOSMYBINP-UHFFFAOYSA-N
Formula:	C18H32O4
SMILES:	CCCCCOC(=O)C1CCCCC1C(=O)OCC(C)C
Mol. weight [g/mol]:	312.44

## Physical Properties

Property code	Value	Unit	Source
gf	-352.86	kJ/mol	Joback Method
hf	-875.75	kJ/mol	Joback Method
hfus	37.33	kJ/mol	Joback Method
hvap	73.71	kJ/mol	Joback Method
log10ws	-4.25		Crippen Method
logp	4.115		Crippen Method
mvol	268.500	ml/mol	McGowan Method
pc	1398.55	kPa	Joback Method
rinpol	2076.00		NIST Webbook
rinpol	2076.00		NIST Webbook
tb	778.26	K	Joback Method
tc	975.02	K	Joback Method
tf	425.08	K	Joback Method
vc	1.018	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	849.26	J/molxK	778.26	Joback Method
cpg	933.07	J/molxK	942.22	Joback Method
cpg	918.79	J/molxK	909.43	Joback Method
cpg	903.28	J/molxK	876.64	Joback Method
cpg	886.53	J/molxK	843.85	Joback Method
cpg	868.53	J/molxK	811.05	Joback Method
cpg	946.13	J/molxK	975.02	Joback Method
dvisc	0.0000852	Paxs	778.26	Joback Method

dvisc	0.0001127	Paxs	719.40	Joback Method
dvisc	0.0001565	Paxs	660.53	Joback Method
dvisc	0.0002320	Paxs	601.67	Joback Method
dvisc	0.0003745	Paxs	542.81	Joback Method
dvisc	0.0006791	Paxs	483.94	Joback Method
dvisc	0.0014522	Paxs	425.08	Joback Method

## Sources

<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=U339427&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U339427&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307l">http://pubs.acs.org/doi/abs/10.1021/ci990307l</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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