

# 1,2-Cyclohexanedicarboxylic acid, hexyl isoheptyl ester

Inchi:	InChI=1S/C20H36O4/c1-4-5-6-9-14-23-19(21)17-12-7-8-13-18(17)20(22)24-15-10-11-16
InchiKey:	MBTKYQHLJXXXGP-UHFFFAOYSA-N
Formula:	C20H36O4
SMILES:	CCCCCOC(=O)C1CCCCC1C(=O)OCCCC(C)C
Mol. weight [g/mol]:	340.50

## Physical Properties

Property code	Value	Unit	Source
gf	-336.02	kJ/mol	Joback Method
hf	-917.03	kJ/mol	Joback Method
hfus	42.51	kJ/mol	Joback Method
hvap	78.16	kJ/mol	Joback Method
log10ws	-5.09		Crippen Method
logp	4.896		Crippen Method
mvol	296.680	ml/mol	McGowan Method
pc	1217.44	kPa	Joback Method
rinpol	2260.00		NIST Webbook
rinpol	2260.00		NIST Webbook
tb	824.02	K	Joback Method
tc	1020.98	K	Joback Method
tf	447.62	K	Joback Method
vc	1.129	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	969.98	J/molxK	824.02	Joback Method
cpg	989.40	J/molxK	856.85	Joback Method
cpg	1007.46	J/molxK	889.67	Joback Method
cpg	1024.18	J/molxK	922.50	Joback Method
cpg	1039.58	J/molxK	955.33	Joback Method
cpg	1053.69	J/molxK	988.16	Joback Method
cpg	1066.50	J/molxK	1020.98	Joback Method
dvisc	0.0011819	Paxs	447.62	Joback Method

dvisc	0.0005412	Paxs	510.35	Joback Method
dvisc	0.0002940	Paxs	573.09	Joback Method
dvisc	0.0001802	Paxs	635.82	Joback Method
dvisc	0.0001206	Paxs	698.55	Joback Method
dvisc	0.0000862	Paxs	761.29	Joback Method
dvisc	0.0000648	Paxs	824.02	Joback Method

## Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=U339410&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U339410&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>cp<sub>g</sub>:</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>log<sub>10</sub>ws:</b>	Log <sub>10</sub> of Water solubility in mol/l
<b>logp:</b>	Octanol/Water partition coefficient
<b>m<sub>c</sub>vol:</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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