

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

Inchi:	InChI=1S/C20H36O4/c1-5-7-8-11-14-23-19(21)16-12-9-10-13-17(16)20(22)24-18(6-2)15
InchiKey:	FXKITTJOEFEUKD-UHFFFAOYSA-N
Formula:	C20H36O4
SMILES:	CCCCCOC(=O)C1CCCCC1C(=O)OC(CC)C(C)C
Mol. weight [g/mol]:	340.50

## Physical Properties

Property code	Value	Unit	Source
gf	-338.46	kJ/mol	Joback Method
hf	-922.31	kJ/mol	Joback Method
hfus	38.99	kJ/mol	Joback Method
hvap	77.77	kJ/mol	Joback Method
log10ws	-5.20		Crippen Method
logp	4.894		Crippen Method
mvol	296.680	ml/mol	McGowan Method
pc	1224.27	kPa	Joback Method
rinpol	2267.00		NIST Webbook
rinpol	2267.00		NIST Webbook
tb	823.58	K	Joback Method
tc	1022.33	K	Joback Method
tf	432.62	K	Joback Method
vc	1.123	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	970.46	J/molxK	823.58	Joback Method
cpg	990.04	J/molxK	856.70	Joback Method
cpg	1008.24	J/molxK	889.83	Joback Method
cpg	1025.07	J/molxK	922.95	Joback Method
cpg	1040.54	J/molxK	956.08	Joback Method
cpg	1054.67	J/molxK	989.20	Joback Method
cpg	1067.49	J/molxK	1022.33	Joback Method
dvisc	0.0014062	Paxs	432.62	Joback Method

dvisc	0.0005879	Paxs	497.78	Joback Method
dvisc	0.0003007	Paxs	562.94	Joback Method
dvisc	0.0001768	Paxs	628.10	Joback Method
dvisc	0.0001149	Paxs	693.26	Joback Method
dvisc	0.0000804	Paxs	758.42	Joback Method
dvisc	0.0000595	Paxs	823.58	Joback Method

## Sources

<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=U339443&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U339443&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>
<b>Crippen Method:</b>	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</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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