

# 1,2-Cyclohexanedicarboxylic acid, hexyl 3-pentyl ester

Inchi:	InChI=1S/C19H34O4/c1-4-7-8-11-14-22-18(20)16-12-9-10-13-17(16)19(21)23-15(5-2)6-3
InchiKey:	FZPYYQKUSRNYBU-UHFFFAOYSA-N
Formula:	C19H34O4
SMILES:	CCCCCOC(=O)C1CCCCC1C(=O)OC(CC)CC
Mol. weight [g/mol]:	326.47

## Physical Properties

Property code	Value	Unit	Source
gf	-344.44	kJ/mol	Joback Method
hf	-896.39	kJ/mol	Joback Method
hfus	39.92	kJ/mol	Joback Method
hvap	75.93	kJ/mol	Joback Method
log10ws	-5.02		Crippen Method
logp	4.648		Crippen Method
mvol	282.590	ml/mol	McGowan Method
pc	1303.29	kPa	Joback Method
rinpol	2133.00		NIST Webbook
rinpol	2133.00		NIST Webbook
tb	801.14	K	Joback Method
tc	997.68	K	Joback Method
tf	436.35	K	Joback Method
vc	1.073	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	909.24	J/molxK	801.14	Joback Method
cpg	993.04	J/molxK	964.93	Joback Method
cpg	978.84	J/molxK	932.17	Joback Method
cpg	963.37	J/molxK	899.41	Joback Method
cpg	946.62	J/molxK	866.65	Joback Method
cpg	928.59	J/molxK	833.90	Joback Method
cpg	1006.00	J/molxK	997.68	Joback Method
dvisc	0.0000744	Paxs	801.14	Joback Method

dvisc	0.0000987	Paxs	740.34	Joback Method
dvisc	0.0001376	Paxs	679.54	Joback Method
dvisc	0.0002048	Paxs	618.75	Joback Method
dvisc	0.0003324	Paxs	557.95	Joback Method
dvisc	0.0006075	Paxs	497.15	Joback Method
dvisc	0.0013131	Paxs	436.35	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=U339504&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U339504&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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