

# 1,2-Cyclohexanedicarboxylic acid, heptyl hexyl ester

Inchi:	InChI=1S/C21H38O4/c1-3-5-7-9-13-17-25-21(23)19-15-11-10-14-18(19)20(22)24-16-12-
InchiKey:	SUKYPVHNNPNNTF-UHFFFAOYSA-N
Formula:	C21H38O4
SMILES:	CCCCCCCOC(=O)C1CCCCC1C(=O)OCCCCC
Mol. weight [g/mol]:	354.52

## Physical Properties

Property code	Value	Unit	Source
gf	-325.16	kJ/mol	Joback Method
hf	-932.39	kJ/mol	Joback Method
hfus	48.63	kJ/mol	Joback Method
hvap	80.77	kJ/mol	Joback Method
log10ws	-5.75		Crippen Method
logp	5.430		Crippen Method
mvol	310.770	ml/mol	McGowan Method
pc	1133.67	kPa	Joback Method
rinpol	2409.00		NIST Webbook
rinpol	2409.00		NIST Webbook
tb	847.34	K	Joback Method
tc	1044.08	K	Joback Method
tf	473.89	K	Joback Method
vc	1.192	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1030.95	J/molxK	847.34	Joback Method
cpg	1050.31	J/molxK	880.13	Joback Method
cpg	1068.30	J/molxK	912.92	Joback Method
cpg	1084.92	J/molxK	945.71	Joback Method
cpg	1100.21	J/molxK	978.50	Joback Method
cpg	1114.17	J/molxK	1011.29	Joback Method
cpg	1126.84	J/molxK	1044.08	Joback Method
dvisc	0.0009131	Paxs	473.89	Joback Method

dvisc	0.0004486	Paxs	536.13	Joback Method
dvisc	0.0002555	Paxs	598.37	Joback Method
dvisc	0.0001618	Paxs	660.62	Joback Method
dvisc	0.0001109	Paxs	722.86	Joback Method
dvisc	0.0000807	Paxs	785.10	Joback Method
dvisc	0.0000615	Paxs	847.34	Joback Method

## Sources

<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=U339537&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U339537&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.cheméo.com/doc/models/crippen_log10ws">https://www.cheméo.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>

## Legend

<b>cp<sub>g</sub>:</b>	Ideal gas heat capacity
<b>dvisc:</b>	Dynamic viscosity
<b>g<sub>f</sub>:</b>	Standard Gibbs free energy of formation
<b>h<sub>f</sub>:</b>	Enthalpy of formation at standard conditions
<b>h<sub>fus</sub>:</b>	Enthalpy of fusion at standard conditions
<b>h<sub>vap</sub>:</b>	Enthalpy of vaporization at standard conditions
<b>log<sub>10</sub>w<sub>s</sub>:</b>	Log <sub>10</sub> of Water solubility in mol/l
<b>log<sub>p</sub>:</b>	Octanol/Water partition coefficient
<b>mc<sub>vol</sub>:</b>	McGowan's characteristic volume
<b>pc:</b>	Critical Pressure
<b>rin<sub>pol</sub>:</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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