

# 1,2-Cyclohexanedicarboxylic acid, heptyl isoheptyl ester

Inchi:	InChI=1S/C21H38O4/c1-4-5-6-7-10-15-24-20(22)18-13-8-9-14-19(18)21(23)25-16-11-12
InchiKey:	XHROFWQSRSEREH-UHFFFAOYSA-N
Formula:	C21H38O4
SMILES:	CCCCCCCOC(=O)C1CCCCC1C(=O)OCCCC(C)C
Mol. weight [g/mol]:	354.52

## Physical Properties

Property code	Value	Unit	Source
gf	-327.60	kJ/mol	Joback Method
hf	-937.67	kJ/mol	Joback Method
hfus	45.10	kJ/mol	Joback Method
hvap	80.38	kJ/mol	Joback Method
log10ws	-5.51		Crippen Method
logp	5.286		Crippen Method
mcvol	310.770	ml/mol	McGowan Method
pc	1139.80	kPa	Joback Method
rinpol	2363.00		NIST Webbook
tb	846.90	K	Joback Method
tc	1044.97	K	Joback Method
tf	458.89	K	Joback Method
vc	1.185	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1031.42	J/molxK	846.90	Joback Method
cpg	1114.96	J/molxK	1011.96	Joback Method
cpg	1100.98	J/molxK	978.95	Joback Method
cpg	1085.66	J/molxK	945.93	Joback Method
cpg	1068.97	J/molxK	912.92	Joback Method
cpg	1050.90	J/molxK	879.91	Joback Method
cpg	1127.60	J/molxK	1044.97	Joback Method
dvisc	0.0000563	Paxs	846.90	Joback Method
dvisc	0.0000751	Paxs	782.23	Joback Method

dvisc	0.0001053	Paxs	717.56	Joback Method
dvisc	0.0001580	Paxs	652.89	Joback Method
dvisc	0.0002591	Paxs	588.23	Joback Method
dvisc	0.0004803	Paxs	523.56	Joback Method
dvisc	0.0010593	Paxs	458.89	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=U339536&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U339536&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>

## 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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