

# 1,2-Cyclohexanedicarboxylic acid, isoheptyl 4-octyl ester

Inchi:	InChI=1S/C22H40O4/c1-5-7-13-18(11-6-2)26-22(24)20-15-9-8-14-19(20)21(23)25-16-10
InchiKey:	YDAYAWZSMYTDGX-UHFFFAOYSA-N
Formula:	C22H40O4
SMILES:	CCCCC(CCC)OC(=O)C1CCCCC1C(=O)OCCCC(C)C
Mol. weight [g/mol]:	368.55

## Physical Properties

Property code	Value	Unit	Source
gf	-321.62	kJ/mol	Joback Method
hf	-963.59	kJ/mol	Joback Method
hfus	44.17	kJ/mol	Joback Method
hvap	82.22	kJ/mol	Joback Method
log10ws	-6.04		Crippen Method
logp	5.674		Crippen Method
mvol	324.860	ml/mol	McGowan Method
pc	1074.98	kPa	Joback Method
rinpol	2311.00		NIST Webbook
rinpol	2311.00		NIST Webbook
tb	869.34	K	Joback Method
tc	1070.39	K	Joback Method
tf	455.16	K	Joback Method
vc	1.236	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1093.91	J/molxK	869.34	Joback Method
cpg	1177.46	J/molxK	1036.88	Joback Method
cpg	1163.65	J/molxK	1003.38	Joback Method
cpg	1148.41	J/molxK	969.87	Joback Method
cpg	1131.72	J/molxK	936.36	Joback Method
cpg	1113.57	J/molxK	902.85	Joback Method
cpg	1189.87	J/molxK	1070.39	Joback Method
dvisc	0.0000447	Paxs	869.34	Joback Method

dvisc	0.0000606	Paxs	800.31	Joback Method
dvisc	0.0000870	Paxs	731.28	Joback Method
dvisc	0.0001348	Paxs	662.25	Joback Method
dvisc	0.0002313	Paxs	593.22	Joback Method
dvisc	0.0004572	Paxs	524.19	Joback Method
dvisc	0.0011117	Paxs	455.16	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=U339520&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U339520&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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