

# cis-Cyclohex-4-en-1,2-dicarboxylic acid, hexyl 3-phenylpropyl ester

Inchi:	InChI=1S/C23H32O4/c1-2-3-4-10-17-26-22(24)20-15-8-9-16-21(20)23(25)27-18-11-14-1
InchiKey:	ZHAPRYDPWHTVQE-UHFFFAOYSA-N
Formula:	C23H32O4
SMILES:	CCCCCOC(=O)C1CC=CCC1C(=O)OCCc1ccccc1
Mol. weight [g/mol]:	372.50

## Physical Properties

Property code	Value	Unit	Source
gf	-165.95	kJ/mol	Joback Method
hf	-679.36	kJ/mol	Joback Method
hfus	49.07	kJ/mol	Joback Method
hvap	87.79	kJ/mol	Joback Method
log10ws	-5.54		Crippen Method
logp	4.868		Crippen Method
mvol	310.890	ml/mol	McGowan Method
pc	1280.08	kPa	Joback Method
rinpol	2720.00		NIST Webbook
tb	918.94	K	Joback Method
tc	1136.69	K	Joback Method
tf	523.61	K	Joback Method
vc	1.181	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1028.16	J/molxK	918.94	Joback Method
cpg	1044.66	J/molxK	955.23	Joback Method
cpg	1059.60	J/molxK	991.52	Joback Method
cpg	1073.02	J/molxK	1027.82	Joback Method
cpg	1084.95	J/molxK	1064.11	Joback Method
cpg	1095.45	J/molxK	1100.40	Joback Method
cpg	1104.55	J/molxK	1136.69	Joback Method
dvisc	0.0006237	Paxs	523.61	Joback Method
dvisc	0.0003268	Paxs	589.50	Joback Method

dvisc	0.0001951	Paxs	655.39	Joback Method
dvisc	0.0001279	Paxs	721.28	Joback Method
dvisc	0.0000900	Paxs	787.16	Joback Method
dvisc	0.0000669	Paxs	853.05	Joback Method
dvisc	0.0000519	Paxs	918.94	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=U382777&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U382777&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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