

# 1,2-Cyclohexanedicarboxylic acid, hexyl 4-isopropylphenyl ester

Inchi:	InChI=1S/C23H34O4/c1-4-5-6-9-16-26-22(24)20-10-7-8-11-21(20)23(25)27-19-14-12-18
InchiKey:	YKYLBMQMSVOTEBH-UHFFFAOYSA-N
Formula:	C23H34O4
SMILES:	CCCCCOC(=O)C1CCCCC1C(=O)Oc1ccc(C(C)C)cc1
Mol. weight [g/mol]:	374.51

## Physical Properties

Property code	Value	Unit	Source
gf	-207.98	kJ/mol	Joback Method
hf	-753.89	kJ/mol	Joback Method
hfus	43.93	kJ/mol	Joback Method
hvap	87.77	kJ/mol	Joback Method
log10ws	-6.27		Crippen Method
logp	5.645		Crippen Method
mcvol	315.190	ml/mol	McGowan Method
pc	1241.58	kPa	Joback Method
rinpol	2694.00		NIST Webbook
rinpol	2661.00		NIST Webbook
rinpol	2661.00		NIST Webbook
tb	924.32	K	Joback Method
tc	1143.98	K	Joback Method
tf	520.37	K	Joback Method
vc	1.190	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1058.09	J/molxK	924.32	Joback Method
cpg	1075.23	J/molxK	960.93	Joback Method
cpg	1090.69	J/molxK	997.54	Joback Method
cpg	1104.50	J/molxK	1034.15	Joback Method
cpg	1116.70	J/molxK	1070.76	Joback Method
cpg	1127.34	J/molxK	1107.37	Joback Method
cpg	1136.43	J/molxK	1143.98	Joback Method

dvisc	0.0006038	Paxs	520.37	Joback Method
dvisc	0.0003045	Paxs	587.69	Joback Method
dvisc	0.0001768	Paxs	655.02	Joback Method
dvisc	0.0001136	Paxs	722.35	Joback Method
dvisc	0.0000787	Paxs	789.67	Joback Method
dvisc	0.0000578	Paxs	856.99	Joback Method
dvisc	0.0000443	Paxs	924.32	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=U339608&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U339608&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307l">http://pubs.acs.org/doi/abs/10.1021/ci990307l</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>mvol:</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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