

# Isophthalic acid, octyl 4-tert-butylcyclohexyl ester

Inchi:	InChI=1S/C26H40O4/c1-5-6-7-8-9-10-18-29-24(27)20-12-11-13-21(19-20)25(28)30-23-1
InchiKey:	FEGDZDGBNXUQAY-UHFFFAOYSA-N
Formula:	C26H40O4
SMILES:	CCCCCCCCOC(=O)c1cccc(C(=O)OC2CCC(C(C)(C)C)CC2)c1
Mol. weight [g/mol]:	416.59

## Physical Properties

Property code	Value	Unit	Source
gf	-177.44	kJ/mol	Joback Method
hf	-819.28	kJ/mol	Joback Method
hfus	47.81	kJ/mol	Joback Method
hvap	93.54	kJ/mol	Joback Method
log10ws	-8.18		Crippen Method
logp	6.966		Crippen Method
mvol	357.460	ml/mol	McGowan Method
pc	1030.59	kPa	Joback Method
rinpol	3131.00		NIST Webbook
rinpol	3131.00		NIST Webbook
tb	990.17	K	Joback Method
tc	1216.23	K	Joback Method
tf	571.60	K	Joback Method
vc	1.353	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1242.76	J/molxK	990.17	Joback Method
cpg	1259.76	J/molxK	1027.85	Joback Method
cpg	1275.06	J/molxK	1065.52	Joback Method
cpg	1288.72	J/molxK	1103.20	Joback Method
cpg	1300.81	J/molxK	1140.87	Joback Method
cpg	1311.42	J/molxK	1178.55	Joback Method
cpg	1320.62	J/molxK	1216.23	Joback Method
dvisc	0.0003390	Paxs	571.60	Joback Method

dvisc	0.0001711	Paxs	641.36	Joback Method
dvisc	0.0000987	Paxs	711.12	Joback Method
dvisc	0.0000628	Paxs	780.88	Joback Method
dvisc	0.0000431	Paxs	850.65	Joback Method
dvisc	0.0000313	Paxs	920.41	Joback Method
dvisc	0.0000238	Paxs	990.17	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=U345740&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U345740&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>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>ws:</b>	Log <sub>10</sub> of Water solubility in mol/l
<b>log<sub>p</sub>:</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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