

# Phthalic acid, isohexyl 2-tert-butyl-6-methylphenyl ester

<b>Inchi:</b>	InChI=1S/C25H32O4/c1-17(2)11-10-16-28-23(26)19-13-7-8-14-20(19)24(27)29-22-18(3)
<b>InchiKey:</b>	YNRWOVREAWBHCV-UHFFFAOYSA-N
<b>Formula:</b>	C25H32O4
<b>SMILES:</b>	<chem>Cc1cccc(C(C)(C)C)c1OC(=O)c1cccc1C(=O)OCCCC(C)C</chem>
<b>Mol. weight [g/mol]:</b>	396.52

## Physical Properties

Property code	Value	Unit	Source
gf	-111.89	kJ/mol	Joback Method
hf	-624.31	kJ/mol	Joback Method
hfus	42.06	kJ/mol	Joback Method
hvap	94.41	kJ/mol	Joback Method
log10ws	-7.44		Crippen Method
logp	6.105		Crippen Method
mcvol	330.470	ml/mol	McGowan Method
pc	1203.96	kPa	Joback Method
rinsol	2687.00		NIST Webbook
tb	988.61	K	Joback Method
tc	1219.80	K	Joback Method
tf	593.65	K	Joback Method
vc	1.250	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1075.53	J/molxK	988.61	Joback Method
cpg	1134.70	J/molxK	1181.27	Joback Method
cpg	1125.42	J/molxK	1142.74	Joback Method
cpg	1114.93	J/molxK	1104.20	Joback Method
cpg	1103.17	J/molxK	1065.67	Joback Method
cpg	1090.05	J/molxK	1027.14	Joback Method
cpg	1142.85	J/molxK	1219.80	Joback Method
dvisc	0.0000198	Paxs	988.61	Joback Method
dvisc	0.0000257	Paxs	922.78	Joback Method

dvisc	0.0000347	Paxs	856.96	Joback Method
dvisc	0.0000491	Paxs	791.13	Joback Method
dvisc	0.0000742	Paxs	725.30	Joback Method
dvisc	0.0001216	Paxs	659.48	Joback Method
dvisc	0.0002224	Paxs	593.65	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=U357096&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U357096&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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