

# Isophthalic acid, decyl hex-3-yl ester

<b>Inchi:</b>	InChI=1S/C24H38O4/c1-4-7-8-9-10-11-12-13-18-27-23(25)20-16-14-17-21(19-20)24(26)
<b>InchiKey:</b>	DFHPTJHGOBPJKF-UHFFFAOYSA-N
<b>Formula:</b>	C24H38O4
<b>SMILES:</b>	CCCCCCCCCOC(=O)c1cccc(C(=O)OC(CC)CCC)c1
<b>Mol. weight [g/mol]:</b>	390.56

## Physical Properties

Property code	Value	Unit	Source
gf	-216.30	kJ/mol	Joback Method
hf	-808.51	kJ/mol	Joback Method
hfus	53.62	kJ/mol	Joback Method
hvap	89.88	kJ/mol	Joback Method
log10ws	-7.93		Crippen Method
logp	6.720		Crippen Method
mcvol	340.140	ml/mol	McGowan Method
pc	1036.57	kPa	Joback Method
rinsol	2835.00		NIST Webbook
tb	932.32	K	Joback Method
tc	1142.37	K	Joback Method
tf	528.50	K	Joback Method
vc	1.313	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1119.86	J/molxK	932.32	Joback Method
cpg	1191.53	J/molxK	1107.36	Joback Method
cpg	1179.81	J/molxK	1072.35	Joback Method
cpg	1166.82	J/molxK	1037.34	Joback Method
cpg	1152.52	J/molxK	1002.34	Joback Method
cpg	1136.88	J/molxK	967.33	Joback Method
cpg	1202.02	J/molxK	1142.37	Joback Method
dvisc	0.0000281	Paxs	932.32	Joback Method
dvisc	0.0000371	Paxs	865.02	Joback Method

dvisc	0.0000513	Paxs	797.71	Joback Method
dvisc	0.0000753	Paxs	730.41	Joback Method
dvisc	0.0001196	Paxs	663.11	Joback Method
dvisc	0.0002108	Paxs	595.80	Joback Method
dvisc	0.0004292	Paxs	528.50	Joback Method

## Sources

<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=U356485&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U356485&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>

## 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>mccvol:</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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