

# Isophthalic acid, hexadecyl 4-methylpent-2-yl ester

Inchi:	InChI=1S/C30H50O4/c1-5-6-7-8-9-10-11-12-13-14-15-16-17-18-22-33-29(31)27-20-19-2
InchiKey:	ZHDORUBQAQSLCT-UHFFFAOYSA-N
Formula:	C30H50O4
SMILES:	CCCCCCCCCCCCCCCCOC(=O)c1cccc(C(=O)OC(C)CC(C)C)c1
Mol. weight [g/mol]:	474.72

## Physical Properties

Property code	Value	Unit	Source
gf	-168.22	kJ/mol	Joback Method
hf	-937.63	kJ/mol	Joback Method
hfus	65.64	kJ/mol	Joback Method
hvap	102.85	kJ/mol	Joback Method
log10ws	-10.20		Crippen Method
logp	8.916		Crippen Method
mcvol	424.680	ml/mol	McGowan Method
pc	740.84	kPa	Joback Method
rinpol	3313.00		NIST Webbook
rinpol	3313.00		NIST Webbook
tb	1069.16	K	Joback Method
tc	1319.32	K	Joback Method
tf	581.12	K	Joback Method
vc	1.643	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1497.17	J/molxK	1069.16	Joback Method
cpg	1570.20	J/molxK	1277.62	Joback Method
cpg	1559.34	J/molxK	1235.93	Joback Method
cpg	1546.71	J/molxK	1194.24	Joback Method
cpg	1532.20	J/molxK	1152.55	Joback Method
cpg	1515.72	J/molxK	1110.85	Joback Method
cpg	1579.37	J/molxK	1319.32	Joback Method
dvisc	0.0000101	Paxs	1069.16	Joback Method

dvisc	0.0000136	Paxs	987.82	Joback Method
dvisc	0.0000195	Paxs	906.48	Joback Method
dvisc	0.0000299	Paxs	825.14	Joback Method
dvisc	0.0000503	Paxs	743.80	Joback Method
dvisc	0.0000962	Paxs	662.46	Joback Method
dvisc	0.0002206	Paxs	581.12	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=U356453&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U356453&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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