

# Isophthalic acid, hexyl tetradecyl ester

**Inchi:** InChI=1S/C28H46O4/c1-3-5-7-9-10-11-12-13-14-15-16-18-23-32-28(30)26-21-19-20-25(27)  
**InchiKey:** BEHGUODIBQXYEO-UHFFFAOYSA-N  
**Formula:** C28H46O4  
**SMILES:** CCCCCCCCCCCCCOC(=O)c1cccc(C(=O)OCCCCC)c1  
**Mol. weight [g/mol]:** 446.66

## Physical Properties

Property code	Value	Unit	Source
gf	-180.18	kJ/mol	Joback Method
hf	-885.79	kJ/mol	Joback Method
hfus	67.50	kJ/mol	Joback Method
hvap	99.17	kJ/mol	Joback Method
log10ws	-9.49		Crippen Method
logp	8.282		Crippen Method
mvol	396.500	ml/mol	McGowan Method
pc	817.26	kPa	Joback Method
rinpol	3370.00		NIST Webbook
rinpol	3370.00		NIST Webbook
tb	1024.28	K	Joback Method
tc	1259.00	K	Joback Method
tf	588.58	K	Joback Method
vc	1.544	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1369.60	J/molxK	1024.28	Joback Method
cpg	1443.70	J/molxK	1219.88	Joback Method
cpg	1432.16	J/molxK	1180.76	Joback Method
cpg	1419.05	J/molxK	1141.64	Joback Method
cpg	1404.30	J/molxK	1102.52	Joback Method
cpg	1387.84	J/molxK	1063.40	Joback Method
cpg	1453.73	J/molxK	1259.00	Joback Method
dvisc	0.0000167	Paxs	1024.28	Joback Method

dvisc	0.0000220	Paxs	951.66	Joback Method
dvisc	0.0000302	Paxs	879.05	Joback Method
dvisc	0.0000440	Paxs	806.43	Joback Method
dvisc	0.0000690	Paxs	733.81	Joback Method
dvisc	0.0001195	Paxs	661.20	Joback Method
dvisc	0.0002368	Paxs	588.58	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=U344713&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U344713&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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