

# Isophthalic acid, heptyl 2-propylphenyl ester

<b>Inchi:</b>	InChI=1S/C24H30O4/c1-3-5-6-7-10-17-27-23(25)20-14-11-15-21(18-20)24(26)28-22-16-
<b>InchiKey:</b>	NUSCMHUTPLLRKN-UHFFFAOYSA-N
<b>Formula:</b>	C24H30O4
<b>SMILES:</b>	CCCCCCCOC(=O)c1cccc(C(=O)Oc2ccccc2CCC)c1
<b>Mol. weight [g/mol]:</b>	382.49

## Physical Properties

Property code	Value	Unit	Source
gf	-111.08	kJ/mol	Joback Method
hf	-578.17	kJ/mol	Joback Method
hfus	50.79	kJ/mol	Joback Method
hvap	93.21	kJ/mol	Joback Method
log10ws	-7.53		Crippen Method
logp	5.986		Crippen Method
mvol	316.380	ml/mol	McGowan Method
pc	1277.33	kPa	Joback Method
rinpol	2865.00		NIST Webbook
rinpol	2865.00		NIST Webbook
tb	964.42	K	Joback Method
tc	1187.99	K	Joback Method
tf	582.44	K	Joback Method
vc	1.212	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1015.71	J/molxK	964.42	Joback Method
cpg	1030.03	J/molxK	1001.68	Joback Method
cpg	1042.95	J/molxK	1038.94	Joback Method
cpg	1054.50	J/molxK	1076.21	Joback Method
cpg	1064.74	J/molxK	1113.47	Joback Method
cpg	1073.72	J/molxK	1150.73	Joback Method
cpg	1081.47	J/molxK	1187.99	Joback Method
dvisc	0.0003008	Paxs	582.44	Joback Method

dvisc	0.0001730	Paxs	646.10	Joback Method
dvisc	0.0001098	Paxs	709.77	Joback Method
dvisc	0.0000752	Paxs	773.43	Joback Method
dvisc	0.0000545	Paxs	837.09	Joback Method
dvisc	0.0000413	Paxs	900.76	Joback Method
dvisc	0.0000325	Paxs	964.42	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=U356630&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U356630&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.cheméo.com/doc/models/crippen_log10ws">https://www.cheméo.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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