

# Isophthalic acid, heptyl 4-isopropylphenyl ester

Inchi:	InChI=1S/C24H30O4/c1-4-5-6-7-8-16-27-23(25)20-10-9-11-21(17-20)24(26)28-22-14-12
InchiKey:	FZVQUCRXTNTDLH-UHFFFAOYSA-N
Formula:	C24H30O4
SMILES:	CCCCCCCOC(=O)c1cccc(C(=O)Oc2ccc(C(C)C)cc2)c1
Mol. weight [g/mol]:	382.49

## Physical Properties

Property code	Value	Unit	Source
gf	-113.52	kJ/mol	Joback Method
hf	-583.45	kJ/mol	Joback Method
hfus	47.27	kJ/mol	Joback Method
hvap	92.82	kJ/mol	Joback Method
log10ws	-7.50		Crippen Method
logp	6.156		Crippen Method
mvol	316.380	ml/mol	McGowan Method
pc	1284.67	kPa	Joback Method
rinpol	3099.00		NIST Webbook
rinpol	3099.00		NIST Webbook
tb	963.98	K	Joback Method
tc	1189.04	K	Joback Method
tf	567.44	K	Joback Method
vc	1.206	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1016.14	J/molxK	963.98	Joback Method
cpg	1030.50	J/molxK	1001.49	Joback Method
cpg	1043.42	J/molxK	1039.00	Joback Method
cpg	1054.95	J/molxK	1076.51	Joback Method
cpg	1065.14	J/molxK	1114.02	Joback Method
cpg	1074.03	J/molxK	1151.53	Joback Method
cpg	1081.66	J/molxK	1189.04	Joback Method
dvisc	0.0003262	Paxs	567.44	Joback Method

dvisc	0.0001776	Paxs	633.53	Joback Method
dvisc	0.0001084	Paxs	699.62	Joback Method
dvisc	0.0000721	Paxs	765.71	Joback Method
dvisc	0.0000511	Paxs	831.80	Joback Method
dvisc	0.0000381	Paxs	897.89	Joback Method
dvisc	0.0000296	Paxs	963.98	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=U344458&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U344458&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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