

# Isophthalic acid, isobutyl 3-methylphenyl ester

<b>Inchi:</b>	InChI=1S/C19H20O4/c1-13(2)12-22-18(20)15-7-5-8-16(11-15)19(21)23-17-9-4-6-14(3)10
<b>InchiKey:</b>	COKBCXQXWAMKBJ-UHFFFAOYSA-N
<b>Formula:</b>	C19H20O4
<b>SMILES:</b>	<chem>Cc1cccc(OC(=O)c2cccc(C(=O)OCC(C)C)c2)c1</chem>
<b>Mol. weight [g/mol]:</b>	312.36

## Physical Properties

Property code	Value	Unit	Source
gf	-155.62	kJ/mol	Joback Method
hf	-480.25	kJ/mol	Joback Method
hfus	34.32	kJ/mol	Joback Method
hvap	81.69	kJ/mol	Joback Method
log10ws	-5.29		Crippen Method
logp	4.027		Crippen Method
mcvol	245.930	ml/mol	McGowan Method
pc	1874.03	kPa	Joback Method
rinpol	2518.00		NIST Webbook
tb	849.58	K	Joback Method
tc	1079.45	K	Joback Method
tf	511.09	K	Joback Method
vc	0.925	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	723.81	J/molxK	849.58	Joback Method
cpg	737.98	J/molxK	887.89	Joback Method
cpg	750.83	J/molxK	926.20	Joback Method
cpg	762.40	J/molxK	964.51	Joback Method
cpg	772.72	J/molxK	1002.83	Joback Method
cpg	781.81	J/molxK	1041.14	Joback Method
cpg	789.70	J/molxK	1079.45	Joback Method
dvisc	0.0005456	Paxs	511.09	Joback Method
dvisc	0.0003141	Paxs	567.50	Joback Method

dvisc	0.0001999	Paxs	623.92	Joback Method
dvisc	0.0001371	Paxs	680.34	Joback Method
dvisc	0.0000996	Paxs	736.75	Joback Method
dvisc	0.0000757	Paxs	793.16	Joback Method
dvisc	0.0000597	Paxs	849.58	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=U344516&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U344516&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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