

# Isophthalic acid, ethyl 2-isopropoxyphenyl ester

<b>Inchi:</b>	InChI=1S/C19H20O5/c1-4-22-18(20)14-8-7-9-15(12-14)19(21)24-17-11-6-5-10-16(17)23
<b>InchiKey:</b>	YIYFMMIVPWKTLV-UHFFFAOYSA-N
<b>Formula:</b>	C19H20O5
<b>SMILES:</b>	CCOC(=O)c1cccc(C(=O)Oc2ccccc2OC(C)C)c1
<b>Mol. weight [g/mol]:</b>	328.36

## Physical Properties

Property code	Value	Unit	Source
gf	-260.62	kJ/mol	Joback Method
hf	-612.47	kJ/mol	Joback Method
hfus	35.51	kJ/mol	Joback Method
hvap	84.10	kJ/mol	Joback Method
log10ws	-5.29		Crippen Method
logp	3.870		Crippen Method
mcvol	251.800	ml/mol	McGowan Method
pc	1846.75	kPa	Joback Method
rinpola	2478.00		NIST Webbook
tb	872.00	K	Joback Method
tc	1100.23	K	Joback Method
tf	533.32	K	Joback Method
vc	0.944	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	750.72	J/molxK	872.00	Joback Method
cpg	804.23	J/molxK	1062.19	Joback Method
cpg	796.26	J/molxK	1024.15	Joback Method
cpg	786.94	J/molxK	986.11	Joback Method
cpg	776.25	J/molxK	948.08	Joback Method
cpg	764.18	J/molxK	910.04	Joback Method
cpg	810.84	J/molxK	1100.23	Joback Method
dvisc	0.0000450	Paxs	872.00	Joback Method
dvisc	0.0000570	Paxs	815.55	Joback Method

dvisc	0.0000746	Paxs	759.11	Joback Method
dvisc	0.0001021	Paxs	702.66	Joback Method
dvisc	0.0001475	Paxs	646.21	Joback Method
dvisc	0.0002286	Paxs	589.77	Joback Method
dvisc	0.0003889	Paxs	533.32	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=U344425&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U344425&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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