

# Isophthalic acid, ethyl 2-ethylbutyl ester

<b>Inchi:</b>	InChI=1S/C16H22O4/c1-4-12(5-2)11-20-16(18)14-9-7-8-13(10-14)15(17)19-6-3/h7-10,12
<b>InchiKey:</b>	HFNHRZCRLQFGPN-UHFFFAOYSA-N
<b>Formula:</b>	C16H22O4
<b>SMILES:</b>	CCOC(=O)c1cccc(C(=O)OCC(CC)CC)c1
<b>Mol. weight [g/mol]:</b>	278.34

## Physical Properties

Property code	Value	Unit	Source
gf	-283.66	kJ/mol	Joback Method
hf	-643.39	kJ/mol	Joback Method
hfus	32.90	kJ/mol	Joback Method
hvap	72.07	kJ/mol	Joback Method
log10ws	-4.23		Crippen Method
logp	3.456		Crippen Method
mvol	227.420	ml/mol	McGowan Method
pc	1829.41	kPa	Joback Method
rinpol	2017.00		NIST Webbook
rinpol	2017.00		NIST Webbook
tb	749.28	K	Joback Method
tc	954.00	K	Joback Method
tf	438.34	K	Joback Method
vc	0.866	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	649.00	J/molxK	749.28	Joback Method
cpg	664.35	J/molxK	783.40	Joback Method
cpg	678.69	J/molxK	817.52	Joback Method
cpg	692.04	J/molxK	851.64	Joback Method
cpg	704.40	J/molxK	885.76	Joback Method
cpg	715.80	J/molxK	919.88	Joback Method
cpg	726.23	J/molxK	954.00	Joback Method
dvisc	0.0009839	Paxs	438.34	Joback Method

dvisc	0.0005289	Paxs	490.16	Joback Method
dvisc	0.0003201	Paxs	541.99	Joback Method
dvisc	0.0002115	Paxs	593.81	Joback Method
dvisc	0.0001494	Paxs	645.63	Joback Method
dvisc	0.0001111	Paxs	697.46	Joback Method
dvisc	0.0000861	Paxs	749.28	Joback Method

## Sources

<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=U356422&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U356422&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>

## Legend

<b>cp<sub>g</sub>:</b>	Ideal gas heat capacity
<b>dvisc:</b>	Dynamic viscosity
<b>g<sub>f</sub>:</b>	Standard Gibbs free energy of formation
<b>h<sub>f</sub>:</b>	Enthalpy of formation at standard conditions
<b>h<sub>fus</sub>:</b>	Enthalpy of fusion at standard conditions
<b>h<sub>vap</sub>:</b>	Enthalpy of vaporization at standard conditions
<b>log<sub>10</sub>w<sub>s</sub>:</b>	Log <sub>10</sub> of Water solubility in mol/l
<b>log<sub>p</sub>:</b>	Octanol/Water partition coefficient
<b>mc<sub>vol</sub>:</b>	McGowan's characteristic volume
<b>pc:</b>	Critical Pressure
<b>rin<sub>pol</sub>:</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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