

# Isophthalic acid, 2-formylphenyl ethyl ester

<b>Inchi:</b>	InChI=1S/C17H14O5/c1-2-21-16(19)12-7-5-8-13(10-12)17(20)22-15-9-4-3-6-14(15)11-18
<b>InchiKey:</b>	YOYKGIOZIUFMLH-UHFFFAOYSA-N
<b>Formula:</b>	C17H14O5
<b>SMILES:</b>	CCOC(=O)c1cccc(C(=O)O)c2ccccc2C=O)c1
<b>Mol. weight [g/mol]:</b>	298.29

## Physical Properties

Property code	Value	Unit	Source
gf	-269.54	kJ/mol	Joback Method
hf	-519.27	kJ/mol	Joback Method
hfus	34.95	kJ/mol	Joback Method
hvap	84.34	kJ/mol	Joback Method
log10ws	-4.46		Crippen Method
logp	2.895		Crippen Method
mvol	219.320	ml/mol	McGowan Method
pc	2374.90	kPa	Joback Method
rinpol	2529.00		NIST Webbook
rinpol	2529.00		NIST Webbook
tb	852.92	K	Joback Method
tc	1086.95	K	Joback Method
tf	545.55	K	Joback Method
vc	0.837	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	621.94	J/molxK	852.92	Joback Method
cpg	667.59	J/molxK	1047.94	Joback Method
cpg	660.78	J/molxK	1008.94	Joback Method
cpg	652.83	J/molxK	969.93	Joback Method
cpg	643.72	J/molxK	930.93	Joback Method
cpg	633.43	J/molxK	891.92	Joback Method
cpg	673.29	J/molxK	1086.95	Joback Method
dvisc	0.0000927	Paxs	852.92	Joback Method

dvisc	0.0001143	Paxs	801.69	Joback Method
dvisc	0.0001452	Paxs	750.46	Joback Method
dvisc	0.0001909	Paxs	699.24	Joback Method
dvisc	0.0002621	Paxs	648.01	Joback Method
dvisc	0.0003800	Paxs	596.78	Joback Method
dvisc	0.0005909	Paxs	545.55	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=U344610&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U344610&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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