

# Isophthalic acid, ethyl 4-methoxybenzyl ester

<b>Inchi:</b>	InChI=1S/C18H18O5/c1-3-22-17(19)14-5-4-6-15(11-14)18(20)23-12-13-7-9-16(21-2)10-8
<b>InchiKey:</b>	SYSFBHHHAOIBFV-UHFFFAOYSA-N
<b>Formula:</b>	C18H18O5
<b>SMILES:</b>	CCOC(=O)c1cccc(C(=O)OCc2ccc(OC)cc2)c1
<b>Mol. weight [g/mol]:</b>	314.33

## Physical Properties

Property code	Value	Unit	Source
gf	-266.60	kJ/mol	Joback Method
hf	-586.55	kJ/mol	Joback Method
hfus	36.44	kJ/mol	Joback Method
hvap	82.26	kJ/mol	Joback Method
log10ws	-4.60		Crippen Method
logp	3.229		Crippen Method
mcvol	237.710	ml/mol	McGowan Method
pc	1994.77	kPa	Joback Method
rinpol	2640.00		NIST Webbook
rinpol	2640.00		NIST Webbook
tb	849.56	K	Joback Method
tc	1077.01	K	Joback Method
tf	537.05	K	Joback Method
vc	0.893	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	693.56	J/molxK	849.56	Joback Method
cpg	706.79	J/molxK	887.47	Joback Method
cpg	718.71	J/molxK	925.38	Joback Method
cpg	729.32	J/molxK	963.28	Joback Method
cpg	738.65	J/molxK	1001.19	Joback Method
cpg	746.68	J/molxK	1039.10	Joback Method
cpg	753.43	J/molxK	1077.01	Joback Method
dvisc	0.0003908	Paxs	537.05	Joback Method

dvisc	0.0002454	Paxs	589.13	Joback Method
dvisc	0.0001661	Paxs	641.22	Joback Method
dvisc	0.0001193	Paxs	693.31	Joback Method
dvisc	0.0000897	Paxs	745.39	Joback Method
dvisc	0.0000700	Paxs	797.47	Joback Method
dvisc	0.0000563	Paxs	849.56	Joback Method

## Sources

<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=U344382&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U344382&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307l">http://pubs.acs.org/doi/abs/10.1021/ci990307l</a>
<b>Crippen Method:</b>	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</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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