

# Isophthalic acid, di(2-ethoxyethyl) ester

<b>Inchi:</b>	InChI=1S/C16H22O6/c1-3-19-8-10-21-15(17)13-6-5-7-14(12-13)16(18)22-11-9-20-4-2/h5
<b>InchiKey:</b>	HRSMYJLYNJFJJP-UHFFFAOYSA-N
<b>Formula:</b>	C16H22O6
<b>SMILES:</b>	CCOCCOC(=O)c1cccc(C(=O)OCCOCC)c1
<b>Mol. weight [g/mol]:</b>	310.34

## Physical Properties

Property code	Value	Unit	Source
gf	-491.22	kJ/mol	Joback Method
hf	-902.55	kJ/mol	Joback Method
hfus	38.80	kJ/mol	Joback Method
hvap	77.28	kJ/mol	Joback Method
log10ws	-2.64		Crippen Method
logp	2.073		Crippen Method
mvol	239.160	ml/mol	McGowan Method
pc	1765.41	kPa	Joback Method
rinpol	2275.00		NIST Webbook
rinpol	2275.00		NIST Webbook
tb	794.56	K	Joback Method
tc	995.40	K	Joback Method
tf	497.80	K	Joback Method
vc	0.907	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	704.14	J/molxK	794.56	Joback Method
cpg	718.49	J/molxK	828.03	Joback Method
cpg	731.79	J/molxK	861.51	Joback Method
cpg	744.01	J/molxK	894.98	Joback Method
cpg	755.15	J/molxK	928.46	Joback Method
cpg	765.19	J/molxK	961.93	Joback Method
cpg	774.12	J/molxK	995.40	Joback Method
dvisc	0.0004351	Paxs	497.80	Joback Method

dvisc	0.0002627	Paxs	547.26	Joback Method
dvisc	0.0001724	Paxs	596.72	Joback Method
dvisc	0.0001207	Paxs	646.18	Joback Method
dvisc	0.0000889	Paxs	695.64	Joback Method
dvisc	0.0000682	Paxs	745.10	Joback Method
dvisc	0.0000540	Paxs	794.56	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=U345856&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U345856&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>cp<sub>g</sub>:</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>log<sub>10</sub>ws:</b>	Log <sub>10</sub> of Water solubility in mol/l
<b>logp:</b>	Octanol/Water partition coefficient
<b>m<sub>c</sub>vol:</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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