

# Isophthalic acid, butyl 2-ethoxyethyl ester

<b>Inchi:</b>	InChI=1S/C16H22O5/c1-3-5-9-20-15(17)13-7-6-8-14(12-13)16(18)21-11-10-19-4-2/h6-8,
<b>InchiKey:</b>	PHCIKHMYGZLEMC-UHFFFAOYSA-N
<b>Formula:</b>	C16H22O5
<b>SMILES:</b>	CCCCOC(=O)c1cccc(C(=O)OCCOCC)c1
<b>Mol. weight [g/mol]:</b>	294.34

## Physical Properties

Property code	Value	Unit	Source
gf	-386.22	kJ/mol	Joback Method
hf	-770.33	kJ/mol	Joback Method
hfus	37.61	kJ/mol	Joback Method
hvap	74.87	kJ/mol	Joback Method
log10ws	-3.56		Crippen Method
logp	2.837		Crippen Method
mvol	233.290	ml/mol	McGowan Method
pc	1790.91	kPa	Joback Method
rinpol	2182.00		NIST Webbook
rinpol	2182.00		NIST Webbook
tb	772.14	K	Joback Method
tc	973.24	K	Joback Method
tf	475.57	K	Joback Method
vc	0.889	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	676.30	J/molxK	772.14	Joback Method
cpg	691.04	J/molxK	805.66	Joback Method
cpg	704.79	J/molxK	839.17	Joback Method
cpg	717.53	J/molxK	872.69	Joback Method
cpg	729.27	J/molxK	906.21	Joback Method
cpg	739.99	J/molxK	939.73	Joback Method
cpg	749.72	J/molxK	973.24	Joback Method
dvisc	0.0006097	Paxs	475.57	Joback Method

dvisc	0.0003602	Paxs	525.00	Joback Method
dvisc	0.0002330	Paxs	574.43	Joback Method
dvisc	0.0001615	Paxs	623.86	Joback Method
dvisc	0.0001181	Paxs	673.28	Joback Method
dvisc	0.0000902	Paxs	722.71	Joback Method
dvisc	0.0000713	Paxs	772.14	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=U345847&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U345847&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>

## 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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