

# Isophthalic acid, ethyl hex-4-yn-3-yl ester

<b>Inchi:</b>	InChI=1S/C16H18O4/c1-4-8-14(5-2)20-16(18)13-10-7-9-12(11-13)15(17)19-6-3/h7,9-11,
<b>InchiKey:</b>	YOGKTBSKCUCDEY-UHFFFAOYSA-N
<b>Formula:</b>	C16H18O4
<b>SMILES:</b>	CC#CC(CC)OC(=O)c1cccc(C(=O)OCC)c1
<b>Mol. weight [g/mol]:</b>	274.31

## Physical Properties

Property code	Value	Unit	Source
gf	-80.86	kJ/mol	Joback Method
hf	-371.09	kJ/mol	Joback Method
hfus	36.02	kJ/mol	Joback Method
hvap	74.22	kJ/mol	Joback Method
log10ws	-4.37		Crippen Method
logp	2.822		Crippen Method
mvol	218.820	ml/mol	McGowan Method
pc	2108.07	kPa	Joback Method
rinpol	2088.00		NIST Webbook
rinpol	2088.00		NIST Webbook
tb	758.28	K	Joback Method
tc	981.87	K	Joback Method
tf	544.44	K	Joback Method
vc	0.828	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	600.93	J/mol×K	758.28	Joback Method
cpg	615.69	J/mol×K	795.54	Joback Method
cpg	629.36	J/mol×K	832.81	Joback Method
cpg	641.97	J/mol×K	870.07	Joback Method
cpg	653.51	J/mol×K	907.34	Joback Method
cpg	664.00	J/mol×K	944.60	Joback Method
cpg	673.45	J/mol×K	981.87	Joback Method

# Sources

<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=U343837&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U343837&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.cheméo.com/doc/models/crippen_log10ws">https://www.cheméo.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>

# Legend

<b>cpg:</b>	Ideal gas heat capacity
<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>rinpola:</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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