

# Isophthalic acid, ethyl 2-methyloct-5-yn-4-yl ester

Inchi:	InChI=1S/C19H24O4/c1-5-7-11-17(12-14(3)4)23-19(21)16-10-8-9-15(13-16)18(20)22-6-2
InchiKey:	LVWSDCWTSNRMU-UHFFFAOYSA-N
Formula:	C19H24O4
SMILES:	CCC#CC(CC(C)C)OC(=O)c1cccc(C(=O)OCC)c1
Mol. weight [g/mol]:	316.39

## Physical Properties

Property code	Value	Unit	Source
gf	-58.04	kJ/mol	Joback Method
hf	-438.29	kJ/mol	Joback Method
hfus	40.27	kJ/mol	Joback Method
hvap	80.51	kJ/mol	Joback Method
log10ws	-5.39		Crippen Method
logp	3.848		Crippen Method
mcvol	261.090	ml/mol	McGowan Method
pc	1655.15	kPa	Joback Method
rinpol	2265.00		NIST Webbook
tb	826.48	K	Joback Method
tc	1045.26	K	Joback Method
tf	563.25	K	Joback Method
vc	0.990	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	769.36	J/molxK	826.48	Joback Method
cpg	784.99	J/molxK	862.94	Joback Method
cpg	799.39	J/molxK	899.41	Joback Method
cpg	812.60	J/molxK	935.87	Joback Method
cpg	824.63	J/molxK	972.33	Joback Method
cpg	835.50	J/molxK	1008.80	Joback Method
cpg	845.22	J/molxK	1045.26	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=U343922&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U343922&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>
<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>h vap:</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>m cvol:</b>	McGowan's characteristic volume
<b>pc:</b>	Critical Pressure
<b>r inpol:</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

Latest version available from:

<https://www.chemeo.com/cid/89-487-4/Isophthalic-acid-ethyl-2-methyloct-5-yn-4-yl-ester.pdf>

Generated by Cheméo on 2024-04-27 19:37:53.686435598 +0000 UTC m=+16535922.607012911.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.