

# Isophthalic acid, butyl trans-hex-3-enyl ester

<b>Inchi:</b>	InChI=1S/C18H24O4/c1-3-5-7-8-13-22-18(20)16-11-9-10-15(14-16)17(19)21-12-6-4-2/h5
<b>InchiKey:</b>	QJWBUTMYQPXRQV-FNORWQNLSA-N
<b>Formula:</b>	C18H24O4
<b>SMILES:</b>	CCC=CCCOC(=O)c1cccc(C(=O)OCCCC)c1
<b>Mol. weight [g/mol]:</b>	304.38

## Physical Properties

Property code	Value	Unit	Source
gf	-184.16	kJ/mol	Joback Method
hf	-562.17	kJ/mol	Joback Method
hfus	41.80	kJ/mol	Joback Method
hvap	76.87	kJ/mol	Joback Method
log10ws	-5.16		Crippen Method
logp	4.157		Crippen Method
mcvol	251.300	ml/mol	McGowan Method
pc	1618.07	kPa	Joback Method
rinpol	2242.00		NIST Webbook
tb	799.64	K	Joback Method
tc	1004.52	K	Joback Method
tf	470.80	K	Joback Method
vc	0.964	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	735.73	J/molxK	799.64	Joback Method
cpg	750.91	J/molxK	833.79	Joback Method
cpg	765.08	J/molxK	867.93	Joback Method
cpg	778.26	J/molxK	902.08	Joback Method
cpg	790.48	J/molxK	936.23	Joback Method
cpg	801.78	J/molxK	970.37	Joback Method
cpg	812.18	J/molxK	1004.52	Joback Method
dvisc	0.0006620	Paxs	470.80	Joback Method
dvisc	0.0003640	Paxs	525.61	Joback Method

dvisc	0.0002241	Paxs	580.41	Joback Method
dvisc	0.0001500	Paxs	635.22	Joback Method
dvisc	0.0001070	Paxs	690.03	Joback Method
dvisc	0.0000803	Paxs	744.83	Joback Method
dvisc	0.0000626	Paxs	799.64	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=U356687&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U356687&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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