

# Isophthalic acid, isohexyl 3-methylbut-2-yl ester

Inchi:	InChI=1S/C19H28O4/c1-13(2)8-7-11-22-18(20)16-9-6-10-17(12-16)19(21)23-15(5)14(3)
InchiKey:	GZXNSKQTDJVZHR-UHFFFAOYSA-N
Formula:	C19H28O4
SMILES:	CC(C)CCCOC(=O)c1cccc(C(=O)OC(C)C(C)C)c1
Mol. weight [g/mol]:	320.42

## Physical Properties

Property code	Value	Unit	Source
gf	-263.28	kJ/mol	Joback Method
hf	-715.87	kJ/mol	Joback Method
hfus	33.62	kJ/mol	Joback Method
hvap	77.97	kJ/mol	Joback Method
log10ws	-5.35		Crippen Method
logp	4.481		Crippen Method
mvol	269.690	ml/mol	McGowan Method
pc	1467.98	kPa	Joback Method
rinpol	2278.00		NIST Webbook
rinpol	2278.00		NIST Webbook
tb	817.04	K	Joback Method
tc	1023.15	K	Joback Method
tf	442.15	K	Joback Method
vc	1.022	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	820.65	J/molxK	817.04	Joback Method
cpg	837.06	J/molxK	851.39	Joback Method
cpg	852.29	J/molxK	885.74	Joback Method
cpg	866.34	J/molxK	920.09	Joback Method
cpg	879.25	J/molxK	954.45	Joback Method
cpg	891.04	J/molxK	988.80	Joback Method
cpg	901.72	J/molxK	1023.15	Joback Method
dvisc	0.0010191	Paxs	442.15	Joback Method

dvisc	0.0004484	Paxs	504.63	Joback Method
dvisc	0.0002364	Paxs	567.11	Joback Method
dvisc	0.0001415	Paxs	629.60	Joback Method
dvisc	0.0000930	Paxs	692.08	Joback Method
dvisc	0.0000655	Paxs	754.56	Joback Method
dvisc	0.0000486	Paxs	817.04	Joback Method

## Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=U344721&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U344721&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</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>
<b>McGowan Method:</b>	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</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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