

# Isophthalic acid, 2-methylbutyl hexyl ester

<b>Inchi:</b>	InChI=1S/C19H28O4/c1-4-6-7-8-12-22-18(20)16-10-9-11-17(13-16)19(21)23-14-15(3)5-2
<b>InchiKey:</b>	FBTXUCSBPOBERQ-UHFFFAOYSA-N
<b>Formula:</b>	C19H28O4
<b>SMILES:</b>	CCCCCOC(=O)c1cccc(C(=O)OCC(C)CC)c1
<b>Mol. weight [g/mol]:</b>	320.42

## Physical Properties

Property code	Value	Unit	Source
gf	-258.40	kJ/mol	Joback Method
hf	-705.31	kJ/mol	Joback Method
hfus	40.67	kJ/mol	Joback Method
hvap	78.75	kJ/mol	Joback Method
log10ws	-5.48		Crippen Method
logp	4.627		Crippen Method
mcvol	269.690	ml/mol	McGowan Method
pc	1450.14	kPa	Joback Method
rinpol	2397.00		NIST Webbook
tb	817.92	K	Joback Method
tc	1019.49	K	Joback Method
tf	472.15	K	Joback Method
vc	1.034	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	819.59	J/molxK	817.92	Joback Method
cpg	888.96	J/molxK	985.89	Joback Method
cpg	877.24	J/molxK	952.30	Joback Method
cpg	864.46	J/molxK	918.70	Joback Method
cpg	850.61	J/molxK	885.11	Joback Method
cpg	835.66	J/molxK	851.51	Joback Method
cpg	899.64	J/molxK	1019.49	Joback Method
dvisc	0.0000577	Paxs	817.92	Joback Method
dvisc	0.0000752	Paxs	760.29	Joback Method

dvisc	0.0001024	Paxs	702.66	Joback Method
dvisc	0.0001472	Paxs	645.03	Joback Method
dvisc	0.0002273	Paxs	587.41	Joback Method
dvisc	0.0003857	Paxs	529.78	Joback Method
dvisc	0.0007448	Paxs	472.15	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=U343792&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U343792&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>mccvol:</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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